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Bounded and inhomogeneous Ising models. II. Specific-heat scaling function for a strip

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The specific heat, energy, and free energy of an infinitely long, square-lattice ferromagnetic Ising strip consisting of n parallel layers with free boundary conditions and a surface magnetic field $H_1 = k_B T h_1$ imposed on the last layer, is analyzed for large n in the light of finite-size scaling theory. It is shown rigorously that the free energy (and, similarly, the energy and specific heat) can be written asymptotically in the scaling form $\Delta f(n,t,h_1) \approx n^{-2}(\ln n) W_1(nt, n^{1/2}h_1) + n^{-2} W_2(nt, n^{1/2}h_1)$, where $t=(T-T_c)/T_c$. The scaling functions $W_i(x,y)$ are computed in explicit closed form and shown to verify all the analyticity and asymptotic requirements anticipated by scaling theory. Furthermore, in the limit $n\to\infty$ at fixed $t \neq 0$, the bulk and surface contributions to the thermodynamic properties are found to account for all except a correction of order $e^{pna/\xi(T)}$, where a is the lattice spacing and $\xi(T)$ is the bulk correlation length; the value of the small rational constant p is interpreted in terms of interference effects between the two opposite boundaries (or "surfaces").

I. INTRODUCTION AND SUMMARY

In this article, we consider a two-dimensional square-lattice Ising model with nearest-neighbor ferromagnetic coupling of strength $J=k_BTK$. We study the free energy and specific heat of a "film" or a strip consisting of n parallel, infinitely long rows of spins, with two free "surfaces" or boundary rows. On one of the boundary rows of this $n\times\infty$ system, a magnetic field $H_1 = k_BTh_1$ is applied. However, no magnetic field acts on the interior spins or on the opposite boundary. When $n\to\infty$, the free energy and specific heat of the film expressed on a per spin basis must become identical with those originally found by Onsager[1] for the bulk, $\infty\times\infty$, two-dimensional square lattice. In particular, the specific heat must diverge logarithmically as $T\to T_c$, since the surface field H_1 can play no role in this limit. However, when n is finite the specific heat of the strip remains a bounded and analytic function of T, although it may display a tall and relatively sharp peak as shown in Fig. 1 (which is based on unpublished calculations by A. E. Ferdinand).

The aim of the present work is to study this crossover, from the smooth analytic behavior to the sharp critical behavior, as a function of the "thickness" or breadth $L=na$ (where a is the lattice spacing). In particular, we will check the finite-size scaling theory of critical behavior initiated by Fisher and Ferdinand,[2] partly tested by them[3] in a discussion of an $m\times n$ square-lattice Ising torus (with periodic boundary conditions), and subsequently developed by Fisher and Barber,[4-7] and Binder and Hohenberg.[8,9] Some exact analyses for the spherical and ideal Bose gas models[10,11] have tested aspects of this theory, but previous exact calculations have not included a surface field, or studied the effect of surfaces on the shift and rounding of the specific-heat peak. (Note that the specific heats in the spherical and ideal Bose models remain bounded even in bulk systems; these models also suffer from physically unrealistic effects associated with the spherical constraint and the constant-density condition, respectively.[5,10])

The surface field H_1 is particularly significant,[6-9] since it enables one to study the magnetization $M_1(T,H_1)$ of the surface layer and the corresponding layer or local susceptibility $\chi_{11} = (\partial M_1/\partial H_1)_T$. In particular, we will test the scaling hypothesis[6-8] involving H_1 and study the subtle features of the corresponding scaling functions.[11]

To explain our results, we summarize the scaling hypothesis for a film: it asserts that the reduced free energy per spin of the film can be written asymptotically as $T\to T_c$, $H_1\to 0$, and $n\to\infty$ in the form

$$\begin{aligned} f(n,t,h_1) &= -F(n,T,H_1)/k_BT \\ &= -\lim_{m\to\infty} F_{nm}(T,H_1)/nmk_BT \\ &\approx t^{2-\alpha} X(L/\xi, h_1/|t|^{\Delta_1}) + f_0(n,T,H_1)\,, \end{aligned} \tag{1.1}$$

where $F_{nm}(T,H_1)$ is the total free energy of a lattice of $n\times m$ spins and

$$t = T/T_c - 1, \quad h_1 = H_1/k_BT\,, \tag{1.2}$$

while $L=na$ is the film thickness. The bulk correlation length, asymptotically given by

$$\xi(T) \approx f^0 a/|t|^{\nu}\,, \tag{1.3}$$

may be defined in terms of the asymptotic decay of the pair spin correlations above T_C, according to

$$\langle s_{\vec{0}} s_{\vec{R}}\rangle \sim e^{-R/\xi(T)}\,, \quad R\to\infty \tag{1.4}$$

in which $s_{\vec{R}} = \pm 1$ denotes a lattice spin located at

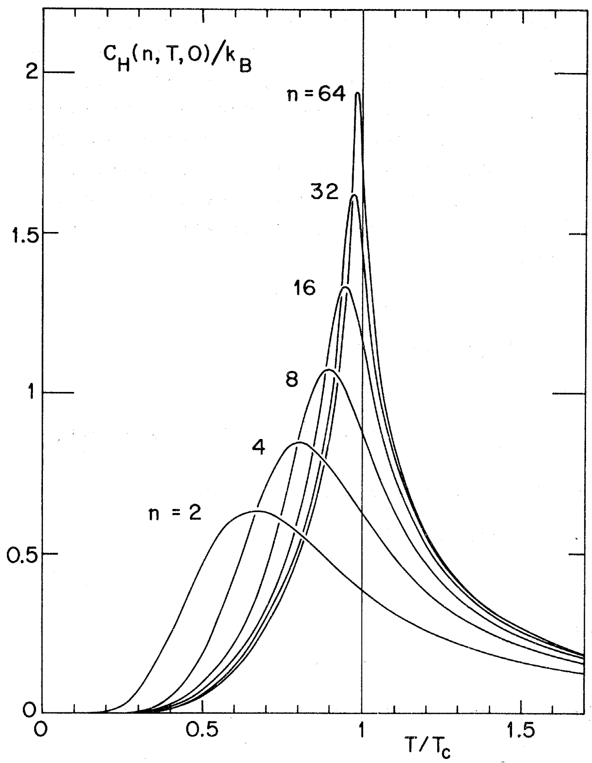

FIG. 1. Specific heat per spin for $n\times\infty$ Ising strips with free edges for $n=2,4,8,16,32$, and 64 (based on calculations by A. E. Ferdinand). It is instructive to compare these curves with those for an $n\times n$ torus (with periodic boundary conditions) shown in Fig. 1 of Ref. 3. Note that the vertical line indicates the location of the divergent logarithmic singularity in the bulk lattice ($n\rightarrow\infty$).

postion $\vec{R}$. The exponent α describes the divergence of the bulk specific heat as $C(T)\sim t^{-\alpha}$, while Δ_1 is a special surface exponent defined in terms of the exponent β_1, which describes the variation of the surface layer magnetization according to $M_1^{\times}(T,0)\sim|t|^{\beta_1}$; the required relation[6–9] is $\Delta_1=2-\alpha-\nu-\beta_1$. The scaling function $X(x,y)$ describes the crossover from bulk to finite-size behavior. Finally, $f_0(n,T,H_1)$ represents the "background" or nonsingular contribution to the free energy, which is uniformly analytic in T and H_1 as $n\rightarrow\infty$. The main physical content of this scaling hypothesis is that, for a "thick" strip ($n\gg1$), the thickness L should enter into the critical behavior *only* via the relation it bears to the correlation length.

In the case of the two-dimensional Ising model we have[12]

$$\alpha=0\ (\log)\ ,\quad \nu=1\ , \tag{1.5}$$

and[13]

$$\beta_1=\tfrac{1}{2}\ ,\quad \text{so that } \Delta_1=\tfrac{1}{2}\ . \tag{1.6}$$

Because of the logarithmic specific heat singularity, the general scaling hypothesis (1.1) must be modified[5] to read

$$\Delta f(n,t,h_1)\approx t^2\ln|t|^{-1}X_1(nt,h_1/t^{1/2}) + t^2X_2(nt,h_1/t^{1/2})\ , \tag{1.7}$$

where $\Delta f=f-f_0$ denotes just the singular part of the free energy. We have also substituted the exponent values (1.5) and (1.6), we have removed the numerical factor $1/f^0$ in replacing L/ξ by nt. [This form for $\alpha=0$ (log) can be anticipated by "borrowing" a term to replace $t^{-\alpha}$ by $(t^{-\alpha}-1)/\alpha$, and letting $\alpha\rightarrow0$.]

The scaling functions $X_1(x,y)$ and $X_2(x,y)$ are subject to restrictions as their arguments attain large or small values. Indeed, one of the purposes of the exact calculations is to check the validity of these restrictions. To elucidate the matter, first note that the free energy of the *finite* width strip should on general grounds, be analytic in t and h_1. Furthermore, the limiting values of these scaling functions should be in agreement with the exact closed-form results of McCoy and Wu,[13] which will form the starting point of our asymptotic analysis.[14]

To impose this analyticity on the scaling form, we may rewrite (1.7) as

$$\Delta f(n,t,h_1)\approx n^{-2}(\ln n)W_1(nt,h_1n^{1/2}) + n^{-2}W_2(nt,h_1n^{1/2})\ , \tag{1.8}$$

where

$$W_1(x,w)=x^2X_1(x,w/x^{1/2}) \tag{1.9}$$

and

$$W_2(x,w)=-x^2\ln|x|X_1(x,w/x^{1/2})+x^2X_2(x,w/x^{1/2})\ . \tag{1.10}$$

Then the theory requires that $W_1(x,w)$ and $W_2(x,w)$ should be analytic functions of x and w.

In the limit when n is very large and T is a fixed distance from T_c, the film should behave as a bulk system with two, independent (infinitely separated) free surfaces. The total free energy as $n\rightarrow\infty$ should then assume the form[5]

$$f(n,t,h_1)=f_\infty(t)+n^{-1}f^{\times}(t,0)+n^{-1}f^{\times}(t,h_1) + O(e^{-pL/\xi})\ , \tag{1.11}$$

where $f_\infty(t)$ denotes the limiting bulk free energy (independent of h_1 as explained) while $f^{\times}(t,h_1)$ is the surface free energy which, of course, depends on h_1. The last, exponentially small term expresses the belief[5,10] that in a film there are no corrections to the bulk free energy per spin beyond those due to the surface, which are proportional to $1/n$; those arising from the "interference" between the two surfaces at separation L are mediated by the correlations, and hence should decay exponentially on a scale set by the correlation length $\xi(T)$. The actual value of the parameter p in (1.11), which may depend on h_1, will be discussed further below in the light of the exact results found in the present calculation. However, one would expect simple integral or fractional values, such as 1, 2, or $\frac{1}{2}$.

To reproduce the asymptotic form (1.11), the scaling functions must, as $x\to\infty$, be of the forms

$$X_i(x,y)=X_i^\infty+x^{-1}X_i^\times(y)+O(e^{-\tilde{p}x}) , \tag{1.12}$$

where $i=1$ or 2 and $\tilde{p}=f^0p$. The singular part of the bulk free energy is then described by

$$\Delta f_\infty(t)\approx X_1^\infty t^2\ln|t|^{-1}+X_2^\infty t^2 , \tag{1.13}$$

as $t\to 0$. Similarly the singular part of the surface free energy is given by

$$\Delta f^\times(t,0)+\Delta f^\times(t,h_1)\approx t\ln|t|^{-1}X_1^\times(h_1/t^{1/2}) + tX_2^\times(h_1/t^{1/2}) , \tag{1.14}$$

for t and h_1 small. Since the surface free energy should be an analytic function when $t\neq 0$, we expect $X_1^\times(y)$ and $X_2^\times(y)$ to be analytic for finite y. Finally, in the opposite limit, where $t=0$ but $h_1\neq 0$, the scaling theory requires that $\Delta f^\times\sim h_1^{-\delta_1+1}\sim h_1^2\ln h_1$, where the scaling relation $-\Delta_1\delta_1=2-\alpha-\nu-\Delta_1=\beta_1$ holds. This yields the restrictions

$$V_1(v)=V_1(y^{-1})=y^{-2}X_1^\times(y)\to V_1^0 \tag{1.15}$$

and

$$V_2(v)=V_2(y^{-1})=2y^{-2}\ln|y|X_1^\times(y)+y^{-2}X_2^\times(y)\to V_2^0 , \tag{1.16}$$

as $y\to\infty$, where V_1^0 and V_2^0 are finite constants.

Our exact analysis bears out all of the above general theory and reveals a number of interesting further details. In particular, we calculate in closed form (given as elementary functions plus integrals over elementary functions) all the various scaling functions $X_i(x,y)$, etc., encountered above. For convenience in dealing with the Ising model, we work explicitly with the *temperature scaling variable*[3]

$$\tau=n(1-\sinh 2K)/(2\sinh 2K)^{1/2} \approx 2K_c nt\sim n(T-T_c) , \tag{1.17}$$

where

$$K=J/k_BT , \quad K_c=\tanh^{-1}(\sqrt{2}-1)\simeq 0.4406868 , \tag{1.18}$$

and the *surface field scaling variable*

$$\sigma=n^{1/2}(1+\sqrt{2})^{1/2}\tanh h_1 \approx k_1 n^{1/2}h_1\sim\sqrt{n}H_1 , \tag{1.19}$$

in which

$$k_1=(1+\sqrt{2})^{1/2}\simeq 1.5537774 . \tag{1.20}$$

Then we may write our main result in the form (1.8) as

$$f(n,t,h_1)\approx n^{-2}\ln n(\tau+\tau^2+\sigma^2)/\pi+n^{-2}Y(\tau,\sigma^2) +n^{-1}D_1+D_0+f_0(n,t,h_1) , \tag{1.21}$$

where the scaling function $Y(\tau,\sigma^2)$, related directly to $W_2(x,w)$, is given by

$$\pi Y(\tau,\sigma^2)=\{\ln 2-\ln[1+(\tau^2+1)^{1/2}]\}(\tau+\tau^2+\sigma^2)-\ln[1+(\tau+\sigma^2)/(\tau^2+1)^{1/2}]+\tau\tan^{-1}(1/\tau)-\tfrac{1}{2}\pi|\tau|+\tfrac{1}{2}\tau^2(1+\ln 2) - (1+\tau^2)^{1/2}+(\tau+\sigma^2)(1+\tfrac{1}{2}\ln 2+\pi/4-\pi/\sqrt{2})-\sigma(\sigma^2+2\tau)^{1/2}\mathcal{L}(\tau,\sigma^2)/\pi+R(\tau,\sigma^2) , \tag{1.22}$$

where

$$\mathcal{L}(\tau,\sigma^2)=\frac{1}{2}\left[\left(1-\frac{|\sigma^2+\tau|}{\sigma^2+\tau}\right)\ln\frac{1+\sigma(\sigma^2+2\tau)^{1/2}}{1-\sigma(\sigma^2+2\tau)^{1/2}}+\ln\frac{(\sigma^2+\tau)+\sigma(\sigma^2+2\tau)^{1/2}}{(\sigma^2+\tau)-\sigma(\sigma^2+2\tau)^{1/2}} -\frac{|\sigma^2+\tau|}{\sigma^2+\tau}\ln\frac{|\sigma^2+\tau|(\tau^2+1)^{1/2}+\tau^2+\sigma(\sigma^2+2\tau)^{1/2}}{|\sigma^2+\tau|(\tau^2+1)^{1/2}+\tau^2-\sigma(\sigma^2+2\tau)^{1/2}}\right] \tag{1.23}$$

and

$$R(\tau,\sigma^2)=\int_0^1 d\xi\,[e^{2X}+e^{-2X}+(\sigma^2+\tau)(e^{2X}-e^{-2X})/X]+\int_1^\infty d\xi\,\{1+[1+(\sigma^2+\tau)/X]^{-1}[1-(\sigma^2+\tau)/X]e^{-4X}\} , \tag{1.24}$$

in which

$$X=(\tau^2+\xi^2)^{1/2} . \tag{1.25}$$

The nonsingular part of the free energy can be written as

$$f_0(n,t,h_1)=\tfrac{1}{2}\ln 2+\tfrac{1}{2}\ln\sinh 2K +n^{-1}(\ln\cosh h_1-\ln\cosh K-\tfrac{1}{2}\ln 2) . \tag{1.26}$$

At the critical point $t=0$, $h_1=0$, the total free energy varies with n as

$$f_c(n)=f(n,0,0)\approx\tfrac{1}{2}\ln 2+D_0+n^{-1}[D_1-\ln(1+\sqrt{2})] +(\pi/48)n^{-2}+\dots , \tag{1.27}$$

where, finally,

$$D_0=\int_0^\pi\frac{d\theta}{2\pi}\ln[2-\cos\theta+(1-\cos\theta)^{1/2}(3-\cos\theta)^{1/2}] =2G/\pi\simeq 0.5831218 \tag{1.28}$$

has been given by Onsager,[1] in which G is Gatalan's constant; while

$$D_1=\int_0^{\pi}\frac{d\theta}{2\pi}\ln\left[1+\sqrt{2}(1-\cos\theta)^{1/2}(3-\cos\theta)^{-1/2}\right]$$
$$\simeq 0.258\,9554\,. \tag{1.29}$$

The reduced energy per spin is given by

$$u(n,t,h_1)=\langle s_{\vec{0}}s_{\vec{\delta}}\rangle\approx -n\left(\frac{\partial f}{\partial\tau}\right)_\sigma$$
$$\approx -(\pi n)^{-1}(\ln n)(1+2\tau)-n^{-1}\left(\frac{\partial Y}{\partial\tau}\right)_\sigma-\left(\frac{\partial f_0}{\partial\tau}\right)_\sigma, \tag{1.30}$$

where $\vec{\delta}$ denotes a nearest-neighbor lattice vector. We may note that higher-order terms enter by differentiating σ with respect to T. At the critical point, we have

$$u_c(n)=u(n,0,0)\approx\tfrac{1}{2}\sqrt{2}-(\pi n)^{-1}\ln n$$
$$-(\pi n)^{-1}(\gamma+3\tfrac{1}{2}\ln 2-\ln\pi-\pi/4)\,, \tag{1.31}$$

where $\gamma\simeq 0.577\,2157$ is Euler's constant.

The specific heat can be expressed explicitly as[3]

$$C_H(n,T,H_1)/k_B=C(n,t,h_1)\approx A_0\ln n+B(\tau,\sigma^2)\,, \tag{1.32}$$

where

$$A_0=(8/\pi)K_c^2=(2/\pi)[\ln(1+\sqrt{2})]^2\simeq 0.494\,5386\,, \tag{1.33}$$

while

$$B(\tau,\sigma^2)=4K_c^2\frac{\partial^2}{\partial\tau^2}Y(\tau,\sigma^2)-2K_c^2\,. \tag{1.34}$$

A more explicit form for $B(\tau,\sigma^2)$ is given in (2.53). Indeed, this was the first form in which the result was obtained. At the critical point, one obtains

$$B_0(0,0)=A_0[\gamma+3\tfrac{1}{2}\ln 2-\ln\pi-14\zeta(3)/\pi^2-\pi/4]$$
$$\simeq -0.312\,5538\,, \tag{1.35}$$

which may be compared with the corresponding result for an infinite torus, which is[3]

$$B_0^{\mathrm{torus}}\simeq 0.187\,9027\,. \tag{1.36}$$

The difference in values of B_0 is evident on comparing Fig. 1 with Fig. 1 of Ref. 3.

The boundary magnetization can be expressed as

$$M_1(n,t,h_1)=\langle s_{\vec{0}}^{1}\rangle=n\left(\frac{\partial f}{\partial h_1}\right)_\tau$$
$$\simeq 2(1+\sqrt{2})h_1\left[\pi^{-1}\ln n+\left(\frac{\partial Y}{\partial\sigma^2}\right)_\tau\right]+h_1\,, \tag{1.37}$$

where $s_{\vec{0}}^{1}$ denotes a spin on the boundary row on which the magnetic field h_1 is applied. One finds that the spontaneous boundary magnetization $M_1(n,t,0^+)$ is identically zero for a finite strip.

Finally, the boundary magnetic susceptibility can be expressed as

$$\chi_{11}(n,t,h_1)=\left(\frac{\partial M_1}{\partial h_1}\right)_\tau\approx(\ln n)2(1+\sqrt{2})/\pi+Z(\tau,\sigma^2)\,, \tag{1.38}$$

in which the scaling function $Z(\tau,\sigma^2)$ is given by

$$Z(\tau,\sigma^2)=2(1+\sqrt{2})\left(\frac{\partial Y}{\partial\sigma^2}\right)_\tau$$
$$+4(1+\sqrt{2})\sigma^2\left(\frac{\partial^2 Y}{\partial(\sigma^2)^2}\right)_\tau+1\,. \tag{1.39}$$

At the critical point itself, one finds

$$\chi_{11}^c(n)=\chi_{11}(n,0,0)=(\ln n)2(1+\sqrt{2})/\pi$$
$$+(\gamma+3\ln 2-\ln\pi)2(1+\sqrt{2})/\pi-\tfrac{1}{2}(\sqrt{2}+1). \tag{1.40}$$

The verification of the analytic properties of the scaling function $Y(\tau,\sigma^2)$ in τ and σ is presented in Sec. III. We also show, in Sec. III, that the large n limit ($\tau\to\infty$) yields the scaling behavior corresponding to the bulk-plus-surface decomposition (1.11). In particular, from (1.32) one obtains the specific heat, for $h_1=0$, as

$$C(n,t,0)\approx A_0(\ln|t|^{-1}-\ln K_c+\tfrac{1}{2}\ln 2-\pi/4)$$
$$+2n^{-1}(-K_c/\pi t)+\dots\,. \tag{1.41}$$

The first term agrees exactly with Onsager's result[1] for the asymptotic behavior of the bulk specific heat $C_\infty(t)$. The second term represents twice the leading behavior of the surface heat $C^\times(t)$, and agrees precisely with the exact result found by Fisher and Ferdinand.[2] The strong divergence as t^{-1} is consistent with (1.5) and the general scaling prediction that surface specific heats should diverge[2,5,7] as $t^{-\alpha-\nu}$.

In Sec. IV we also show that the scaling form of the corrections

$$n^{-2}e(n,t,h_1)=f(n,t,h_1)-f_\infty$$
$$-n^{-1}[f^\times(t,0)+f^\times(t,h_1)] \tag{1.42}$$

to the bulk-plus-surface behavior of the free energy, are given for $h_1=0$ and $T>T_c$ by

$$e(n,t,0)\approx E_0^+(\tau)e^{-4\tau}+O(e^{-4\tau}/\tau^{3/2}) \tag{1.43}$$

as $\tau\to\infty$, with $E_0^+(\tau)=1/32(2\pi\tau)^{1/2}$. This confirms the theoretical form anticipated above. Since one has[1,12]

$$L/\xi(\tau)\approx 2\tau\quad(T>T_c)\,, \tag{1.44}$$

the parameter p in (1.12) is equal to 2. This may be understood, when it is recalled that the energy-energy correlations $\langle s_{\vec{0}}s_{\vec{\delta}}s_{\vec{R}}s_{\vec{R}+\vec{\delta}}\rangle$ decay as $e^{-2R/\xi}$, i.e., as the *square* of the spin-spin correlations $\langle s_{\vec{0}}s_{\vec{R}}\rangle$.[15,16] (This in turn can be seen diagramatically in the high-temperature expansion in powers of $v=\tanh K$, since the leading long-distance contribution to $\langle s_{\vec{0}}s_{\vec{R}}\rangle$ consists of a chain of bonds from $\vec{0}$ to $\vec{R}$, but the energy-energy correlation requires two similar chains to reach the same distance.) Now the spatial integral (or sum) of the energy-energy correlations is, of course, just the total specific heat, which is thus expected to contain terms of order $e^{-2L/\xi}=e^{-4\tau}$. Integration of the specific heat (at constant $L=na$) yields the free energy, which should thus also exhibit similar n-dependent corrections, as indeed observed.

In the presence of a nonzero magnetic field h_1, above T_c, the form (1.43) still applies but with $E_0^+(\tau)$ replaced by a function $E^+(\sigma^2, \tau)$, with $E^+(0,\tau) = E_0^+(\tau)$. Since the field H_1 is applied only to a single surface, this is consistent with our previous interpretation. However, had a field been applied to both surfaces one would expect the spin-spin correlation function to come into play (along with single chain diagrams stretching across the film), so that corrections of order $e^{-L/\xi}=e^{-2\tau}$ should appear.

For $T<T_c$, the asymptotic behavior is quite different: more explicitly, for zero field, $h_1=0$, one finds

$$e(n, t, 0)=2|\tau|e^{-2|\tau|}+O(e^{-2|\tau|}) . \qquad (1.45)$$

But for $T<T_c$, one has (for the net correlation function $\langle s_0^\ast s_R^\ast\rangle - \langle s_0^\ast s_\infty^\ast\rangle$) the result[1,12]

$$L/\xi(T)\approx 4\tau \quad (T<T_c) . \qquad (1.46)$$

Thus the correction is *larger* than the expected $e^{-L/\xi}=e^{-4|\tau|}$, and the parameter p in (1.12) is only $\frac{1}{2}$. At first sight this slower decay of the surface-to-surface interference term is quite puzzling. However, the presence of a (single) surface field H_1 removes this slow decay and yields instead

$$e(n, t, h_1)\approx E^-(\sigma^2, \tau)e^{-4|\tau|} , \quad (h_1\neq 0) \qquad (1.47)$$

as $\tau\to\infty$. This now has the decay expected on the basis of the previous energy-energy correlation arguments, since, below T_c, both *spin* and *energy* correlations[15,16] decay as $e^{-L/\xi}=e^{-4|\tau|}$, leading to $p=1$. As $\sigma\sim h_1\to 0$, the function $E^-(\sigma^2,\tau)$ (which is given explictly below in Sec. IV), diverges so that the more complete expression must be used and (1.45) results.

The removal of the slowly decaying interference term by the surface field suggests that its role is to stabilize the magnetization of the film in, say, the "up" direction. In a thick film, long-range order would set in below T_c, and with overwhelming probability the whole sample would point up, provided h_1 is not too small. When $h_1\to 0$, the film may break up into two or more domains spontaneously magnetized in opposite directions and separated by a fluctuating domain wall or interface. The shortest domain walls will be those of length $\approx L$, which stretch *across* the film from one boundary to the other. Such a wall has a free energy $\Sigma(T)$ per unit length. The probability of a single wall dividing the strip into one "up" and one "down" domain, is thus proportional to $e^{-L\Sigma}$. However, the exact results[1,2,17] show that the interfacial free energy varies as

$$\Sigma(T)\approx 4(K-K_c)/a\approx 2|\tau|/L \quad (T<T_c) . \qquad (1.48)$$

In conclusion, then, we may, when $h=0$ below T_c, expect corrections to the free energy which decay as $e^{-2|\tau|}$, just as found in (1.45). Note that as soon as $h_1\neq 0$ a "down" domain stretching over half the strip becomes improbable, because of the large energy ($\sim h_1\times\infty$) associated with the field acting on the domain at the surface. Diagramatically, below T_c the interfacial free energy is described in leading order by a chain of bonds, but the spin-spin, and all other correlations of local quantities require two similar, but nonintersecting chains. This provides an understanding of the difference between (1.41) and (1.44), and of the result $p=\frac{1}{2}$.

Finally, in summarizing our results, we discuss the numerical form of the specific heat in more detail. In Fig. 2, we plot, for $\sigma=h_1=0$,

$$B(\tau, 0)-B(0, 0)\approx C(n, t, 0)-C(n, 0, 0) , \qquad (1.49)$$

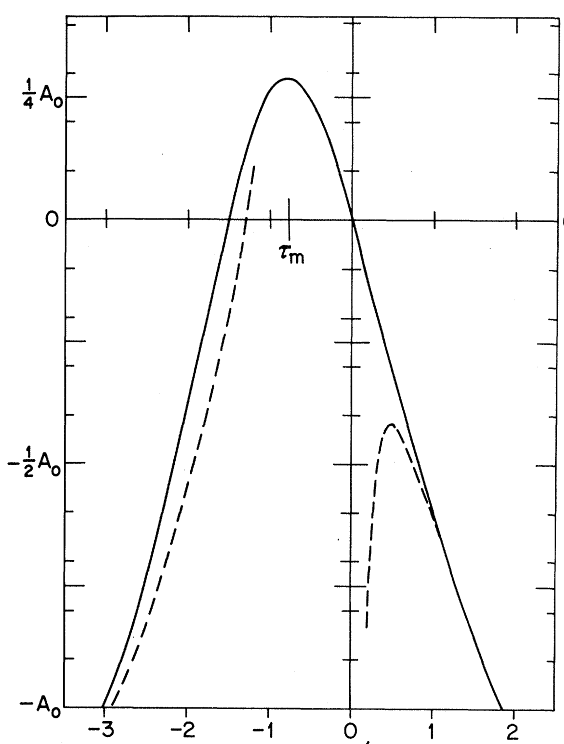

FIG. 2. The asymptotic specific heat of a finite strip $B(\tau,0)-B(0,0)\approx C(n,t,0)-C(n,0,0)$, relative to its critical value $C_c(n)=C(n,0,0)$ vs the reduced temperature variable $\tau\sim n\Delta T/T_c$ (solid curve), and the reduced specific heat of a semiinfinite Ising lattice $\tilde{B}(\tau)=C_\infty(t)+2n^{-1}C^\times(t)-C_c(n)$, relative to $C_c(n)$ (broken curves) in units of $A_0=(2/\pi)[\ln(1+\sqrt{2})]^2\simeq 0.494358$.

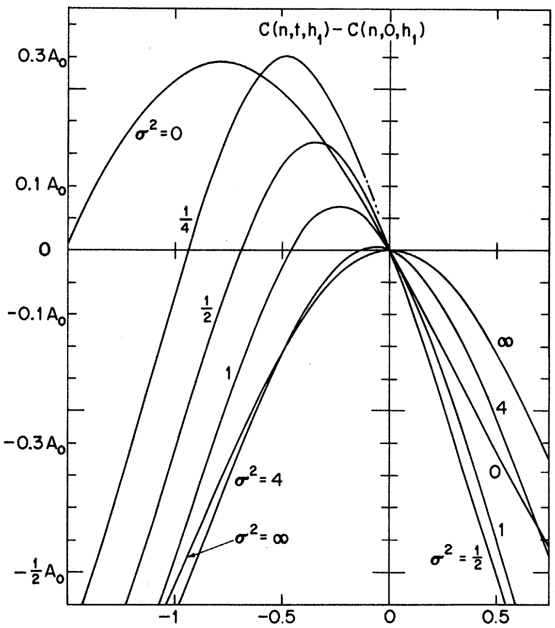

FIG. 3. Plots of the asymptotic field-dependent specific heat $B(\tau, \sigma^2) - B(0, \sigma^2) \approx C(n, t, h_1) - C(n, 0, h_1)$, relative to its value $C(n, 0, h_1)$ at $T = T_c$ vs τ, for $\sigma^2 = (1+\sqrt{2})nh_1^2 = 0, \frac{1}{2}, 1, 4$, and ∞, in units of A_0.

which represents the asymptotically rounded form of the specific heat relative to its finite critical point value $C_c(n) \approx C(n, 0, 0)$. Also shown in the figure is the difference

$$\tilde{B}(\tau) = C_\infty(t) + 2n^{-1}C^\times(t) - C(n, 0, 0)\,, \qquad (1.50)$$

which represents the contributions to $B(\tau, 0)$ of the bulk and surface specific heats [as given by (1.41)]. As expected, the two curves coincide asymptotically for large τ ($n \to \infty$). A striking feature of Figs. 1 and 2 is that the specific-heat maximum is displaced below T_c to the point

$$\tau_m \simeq -0.786\,8771\,. \qquad (1.51)$$

This means that the fractional shift in the pseudocritical point,[3,5,7]

$$\epsilon = 1 - T_{\max}(n)/T_c \approx -c/t^\lambda\,, \qquad (1.52)$$

is described for $h_1 = 0$ by

$$\lambda = 1/\nu = 1\,, \quad c \simeq 0.892\,7850\,. \qquad (1.53)$$

The first exponent relation again confirms the scaling predictions.[2,5,7] On the basis of a numerical study of small finite strips Fisher has estimated[5] $c \simeq 0.900 \pm 0.007$, which compares quite well with our results. (This estimate utilized unpublished numerical work by A. E. Ferdinand and M. N. Barber.)

The curves in Fig. 3 show the effects of imposing the surface field H_1. The predominant feature is that the maximum in the specific heat moves closer to T_c as the field increases. This is intuitively correct since the field aligns the spins near the surface, which, in turn, then tend to align themselves and nearby interior spins more strongly. An argument based on the Griffiths inequalities[18] strengthens this intuitive approach. By setting to zero the interactions between the nth and $(n-1)$th rows, and with the field h_1 acting on the first row, an $n \times \infty$ strip is reduced to an $(n-1) \times \infty$ strip. The Griffiths inequalities then suggest that the ordering temperature $T_{\max}$ satisfies the relation: $T_{\max}(n, h_1) > T_{\max}(n-1, h_1)$. But via the scaling relation, we have $T_{\max}(n-1, h_1) \approx T_{\max}(n, h_1')$, where $h_1' = h_1(n-1)^{1/2}/n^{1/2} \approx h_1(1 - \frac{1}{2}n^{-1}) < h_1$. Thus, we conclude that $T_{\max}(n, h_1) > T_{\max}(n, h_1')$ for $h_1 > h_1'$.

In the limit $h_1 \to \infty$, one finds that the fractional shift ϵ vanishes to the order $n^{-\lambda} = n^{-1}$. (Of course there are still higher-order corrections which we have not elucidated.) Ferdinand and Fisher[3] found a similar result for an infinitely long torus with periodic boundary condition ($\xi = n/m \to \infty$ in their notation[3]). In Fig. 4, we compare their result with ours for two free surfaces on one of which the spins are fully aligned ($h_1 = \infty$); the two curves coincide asymptotically for large τ. This is an expected result for the following reason. In the limit that τ is very large, the film should behave as a

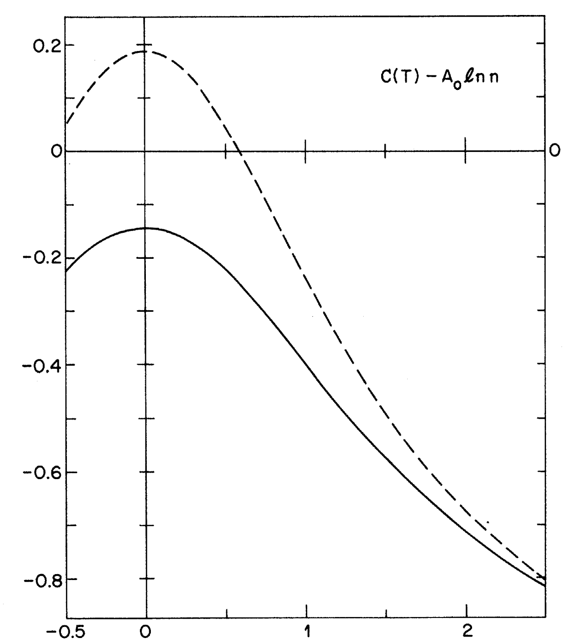

FIG. 4. Comparison between the asymptotic specific heat of an infinitely long, $n \times \infty$ torus (dashed curve), and of an Ising strip with two surfaces, on one of which the spins are fully aligned (solid curve), relative to $A_0 \ln n$. (The curves are symmetric about $\tau = 0$ and asympototically equal as $\tau \to \infty$.)

bulk system, plus a free surface, and a ferromagnetic surface. It was found by Ferdinand and Fisher[2] that the leading term of the surface specific heat for a ferromagnetic wall is

$$C^{\times}_{\text{ferro}} \sim K_c/\pi t \, , \tag{1.54}$$

while, for a free boundary, it is

$$C^{\times}_{\text{free}} \sim -K_c/\pi t \, . \tag{1.55}$$

Consequently, the total surface specific heat vanishes identically! Thus for large τ, the film behaves as a bulk system when $h_1=\infty$. Since there is no surface free energy for a Ising torus, it also should behave as a bulk system when τ is large. This means that the two curves, which are symmetric about the point $\tau=0$, should coincide asymptotically for large τ.

In the remainder of the article we establish the asymptotic results quoted here, starting with the exact expression of McCoy and Wu[13,14] for the free energy of a $n\times\infty$ strip with a field H_1 imposed on one boundary. The arguments are quite intricate in places so that various details have been relegated to appendices. The main analysis is performed in Sec. II. In Sec. III, the properties of the scaling function are studied, and Sec. IV is devoted to the correction term to the bulk plus surface behavior for large τ.

II. FREE ENERGY

We consider a $n\times\infty$ Ising strip with magnetic field H_1 applied on the first row. The reduced free energy per spin will be written

$$\begin{aligned} f(n,t,h_1) &= \lim_{m\to\infty} (2mn)^{-1}\ln Z \\ &= f_0(n,T,H_1)+\Delta f(n,t,h_1) \, , \end{aligned} \tag{2.1}$$

where Z is the partition function. The nonsingular contribution to the free energy as given by McCoy and Wu.[13] is

$$f_0(n,T,H_1)=\tfrac{1}{2}\ln 2+\tfrac{1}{2}\ln\sinh 2K+n^{-1}(\ln\cosh h_1-\ln\cosh K-\tfrac{1}{2}\ln 2) \, , \tag{2.2}$$

where the singular part of the free energy, Δf, can be written as

$$\Delta f(n,t,h_1)=\frac{1}{\pi n}\int_0^1 \frac{d\omega}{(1-\omega^2)^{1/2}}\ln[\lambda_+^n v_+ +\lambda_-^n v_- + z^2 u(\lambda_+^n-\lambda_-^n)] \, , \tag{2.3}$$

in which,

$$\lambda_\pm(\omega)=(1+2\tau^2 n^{-2}+2\omega^2)\pm 2(\tau^2 n^{-2}+\omega^2)^{1/2}(1+\tau^2 n^{-2}+\omega^2)^{1/2} \tag{2.4}$$

and

$$v_\pm(\omega)=1\pm(\tau^2 n^{-2}+1)^{1/2}\{\tau n^{-1}+\omega^2[(\tau^2 n^{-2}+2)^{1/2}-\tau n^{-1}]\}(\tau^2 n^{-2}+\omega^2)^{-1/2}(1+\tau^2 n^{-2}+\omega^2)^{-1/2} \, ; \tag{2.5}$$

we also have

$$z=\tanh h_1 \tag{2.6}$$

and

$$u(\omega)=(1-\omega^2)\{1+(\tau^2 n^{-2}+1)^{1/2}[(\tau^2 n^{-2}+2)^{1/2}-\tau n^{-1}]\}(\tau^2 n^{-2}+\omega^2)^{-1/2}(1+\tau^2 n^{-2}+\omega^2)^{-1/2} \, . \tag{2.7}$$

The *scaled temperature variable* τ was defined in (1.17). The differences of notation between this article and McCoy and Wu's[13] are outlined in Appendix A.

It is evident from (2.4) that $\lambda_+(\omega)>\lambda_-(\omega)$ for $T\neq T_c$. Hence when $n\to\infty$, $T\neq T_c$, the term $\lambda_-^n(\omega)$ in (2.3) is negligible compared to $\lambda_+^n(\omega)$; this yields

$$\Delta f \approx \frac{1}{\pi}\int_0^1 \frac{d\omega}{(1-\omega^2)^{1/2}}\ln\lambda_+ + \frac{1}{\pi n}\int_0^1 \frac{d\omega}{(1-\omega^2)^{1/2}}\ln v_+ \, . \tag{2.8}$$

The first term here gives the bulk free energy $f_\infty(\tau)$, and one finds[1] for T near T_c that $f_\infty(T) \sim t^2\ln|t|$; the second integral gives the surface free energy[13] $f^\times(T,h_1)$ with $f^\times(\tau)\sim t\ln|t|$ for $t\to 0$. However for a finite strip, n is finite and one can no longer drop the λ_-^n term. We shall now show that the "singular" part of the free energy, Δf, for a *finite* strip, given by (2.3), is in fact, analytic. The integrand of Δf can be written as

$$\ln\{\lambda_+^n+\lambda_-^n+(\lambda_+^n-\lambda_-^n)[\tfrac{1}{2}(v_+-v_-)+z^2 u]\} \, . \tag{2.9}$$

One finds, from (2.6) and (2.7), that

$$z^2 u(\omega)\geqslant 0 \quad \text{for} \quad \omega\in[0,1] \, , \tag{2.10}$$

and, by (2.5), we have

$$|\tfrac{1}{2}(v_+-v_-)|\leqslant 1 \quad \text{or} \quad \tfrac{1}{2}[v_+(\omega)-v_-(\omega)]\geqslant -1 \, . \tag{2.11}$$

On combining the above two inequalities, we get

$$\lambda_+^n+\lambda_-^n+(\lambda_+^n-\lambda_-^n)[\tfrac{1}{2}(v_+-v_-)+z^2 u]\geqslant 2\lambda_-^n \, . \tag{2.12}$$

Since $\lambda_-(\omega)>0$ for all ω and τ, this shows that the argument of the logarithm in (2.9) is positive. We shall next show that it is an analytic function of τ and ω. It can be seen from (2.4) that $\lambda_+(\omega)-\lambda_-(\omega)$

contains the singular term $(\tau^2 n^{-2}+\omega^2)^{1/2}$. The first term of the argument $\lambda_+^n+\lambda_-^n$ contains only even powers of $\lambda_+(\omega)-\lambda_-(\omega)$. Hence it is analytic. The second term is a product of $(\lambda_+^n-\lambda_-^n)$ and $[\frac{1}{2}(v_+-v_-)+z^2u]$. Because $\lambda_+^n-\lambda_-^n$ contains only odd terms in $(\lambda_+-\lambda_-)$, and $[\frac{1}{2}(v_+-v_-)+z^2u]$ contains $(\tau^2n^{-2}+\omega^2)^{1/2}$ in its denominator, one concludes that the second term is also analytic. Since the argument of the logarithm in (2.9) has been shown to be positive and analytic, we find the integrand of (2.3) is an analytic function of τ and ω. This means the free energy of an finite strip is an analytic function of T, as it is to be expected on general grounds.

Consider now the ratio $\lambda_-/\lambda_+=\lambda_-^2(\omega)=\lambda_+^{-2}(\omega)$. Since $\lambda_+(\omega)$ of (2.4) is an increasing function of ω, this ratio is a decreasing function of ω. For $\omega\approx c/n\leqslant 1$, we find

$$e^{-n\xi(\omega)}=(\lambda_-/\lambda_+)^n \tag{2.13}$$

$$\approx[1-2(\tau^2+c^2)^{1/2}n^{-1}]^{2n}\approx\exp[-4(\tau^2+c^2)^{1/2}]\approx e^{-4c}\ . \tag{2.14}$$

We shall choose c, such that $c\gg 1$, so that e^{-4c} is negligible. A suitable choice proves to be $c=n^{1/2}$. This means that when ω is larger than c/n or of the order of c/n, the ratio $(\lambda_-/\lambda_+)^n=e^{-n\xi}$ is negligible. For this reason, we separate the interval of integration into two parts $[0,c/n]$ and $[c/n,1]$. In the interval $[c/n,1]$, the ratio $(\lambda_-/\lambda_+)^n$ is initially neglected, and so the basic expression (2.3) can be written

$$\Delta f(n,t,h_1)=I_1+I_2+I_3+E_1\ , \tag{2.15}$$

where

$$I_1=\pi^{-1}\int_0^1\frac{d\omega}{(1-\omega^2)^{1/2}}\ln\lambda_+(\omega)\ , \tag{2.16}$$

$$I_2=(\pi n)^{-1}\int_0^{c/n}\frac{d\omega}{(1-\omega^2)^{1/2}}\times\ln[v_++v_-e^{-n\xi}+z^2u(1-e^{-n\xi})]\ , \tag{2.17}$$

and

$$I_3=(\pi n)^{-1}\int_{c/n}^1\frac{d\omega}{(1-\omega^2)^{1/2}}\ln\,(v_++z^2u)\ . \tag{2.18}$$

The correction term

$$E_1=(\pi n)^{-1}\int_{c/n}^1\frac{d\omega}{(1-\omega^2)^{1/2}}\times\{\ln[v_++v_-e^{-n\xi}+z^2u(1-e^{-n\xi})]-\ln(v_++z^2u)\} \tag{2.19}$$

can rigorously be shown to be of the order e^{-4c} (see Appendix B). The function $\lambda_+(\omega)$ in (2.16), defined by (2.4), a singular at the origin $\omega=0$ for $\tau=0$. Therefore, the dominant contribution to I_1, comes from the interval where ω is small. For small ω, the integrand of I_1 behaves as $2(\tau^2n^{-2}+\omega^2)^{1/2}$. Let us therefore write

$$I_1=\pi^{-1}\int_0^1 d\omega\,2(\tau^2n^{-2}+\omega^2)^{1/2}+\pi^{-1}\Sigma_1(\tau n^{-1})\ . \tag{2.20}$$

It is shown in Appendix C that the function

$$\Sigma_1(\tau n^{-1})=\int_0^1 d\omega\,(1-\omega^2)^{-1/2}\ln\lambda_+ -2\int_0^1 d\omega\,(\tau^2n^{-2}+\omega^2)^{1/2} \tag{2.21}$$

is well behaved, and has the asymptotic expansion

$$\pi^{-1}\Sigma_1(\tau n^{-1})=D_0+\tfrac{1}{2}\tau^2n^{-2}D_2+O(1/nc^3\ ,\ c^2/n^4)\ , \tag{2.22}$$

with

$$\pi D_0=\Sigma_1(0)=\int_0^1 d\omega\,(1-\omega^2)^{-1/2}\ln[1+2\omega^2+2\omega(1+\omega^2)^{1/2}]-1$$
$$=2G-1\simeq 0.831\,931\,188\ , \tag{2.23}$$

where G is Catalan's constant, and

$$\pi D_2=\Sigma_1''(0)=2\int_0 d\omega\,\omega^{-1}[(1-\omega^4)^{-1/2}-1]=\ln 2\ . \tag{2.24}$$

The integral in (2.20) can be written as a sum of two integrals, namely,

$$I_1-\pi^{-1}\Sigma_1(\tau n^{-1})=2\pi^{-1}\int_0^{1/n}d\omega\,(\tau^2n^{-2}+\omega^2)^{1/2}+2\pi^{-1}\int_{1/n}^1 d\omega\,(\tau^2n^{-2}+\omega^2)^{1/2}\ . \tag{2.25}$$

The second integral can be performed, and is

$$\int_{1/n}^1 d\omega\,2(\tau^2n^{-2}+\omega^2)^{1/2}=1+\tau^2n^{-2}\ln n+n^{-2}P(\tau)\ , \tag{2.26}$$

in which

$$P(\tau)=\tfrac{1}{2}\tau^2-(1+\tau^2)^{1/2}+\tau^2\{\ln 2-\ln[(\tau^2+1)^{1/2}+1]\}\ . \tag{2.27}$$

Substituting (2.22) and (2.26) into (2.25), we get

$$I_1=\pi^{-1}n^{-2}\int_0^1 d\xi\,2(\tau^2+\xi^2)^{1/2}+(\tau^2/\pi)n^{-2}\ln n+\pi^{-1}n^{-2}P(\tau)+2G/\pi+\tfrac{1}{2}\tau^2n^{-2}\pi^{-1}\ln 2+O(n^{-5/2})\ , \tag{2.28}$$

where $\xi=n\omega$, and following (2.22), we have choser $c=n^{1/2}$ to optimize the error term.

Analogously, the function $v_+(\omega)+z^2u(\omega)$ in I_3 is singular for $\omega=0$ and $\tau=0$. When ω is small, we have

$$v_+(\omega)+z^2u(\omega)\approx 1+(\tau+\sigma^2)(\tau^2+n^2\omega^2)^{-1/2}\ , \tag{2.29}$$

in which, recapitulating (1.19), we introduce the scaled surface-field variable

$$\sigma=n^{1/2}(1+\sqrt{2})^{1/2}\tanh h_1\ .$$

Hence, we write

$$I_3 = \pi^{-1}n^{-1}\int_{c/n}^{1} d\omega \ln[1+(\tau+\sigma^2)(\tau^2+n^2\omega^2)^{-1/2}] + \pi^{-1}n^{-1}\Sigma_2(\tau n^{-1}, \sigma^2 n^{-1}) . \tag{2.30}$$

On expanding $\Sigma_2(\tau n^{-1}, \sigma^2 n^{-1})$ as a function of n^{-1}, and following arguments similar to those used in Appendix C (which we will not present in detail) one finds,

$$\pi^{-1}\Sigma_2(\tau n^{-1}, \sigma^2 n^{-1}) = D_1 + n^{-1}(\sigma^2+\tau)D_3 + E_3 + O(n^{-5/2}) , \tag{2.31}$$

where

$$\pi D_1 = \Sigma_2(0,0) = \int_0^1 d\omega\,(1-\omega^2)^{-1/2}\ln[1+\sqrt{2}\,\omega(1+\omega^2)^{1/2}] \simeq 0.813\,532\,308 \tag{2.32a}$$

and

$$\pi D_3 = \int_0^1 d\omega\,\omega^{-1}[(1+\omega^2)^{1/2}(1-\omega^2)^{-1/2}-1] - \sqrt{2}\int_0^1 d\omega\,(1-\omega^2)^{-1/2} = \tfrac{1}{2}\ln 2 + \tfrac{1}{2}(\tfrac{1}{2}-\sqrt{2})\pi , \tag{2.32b}$$

with

$$E_3 = -\int_0^{c/n} d\omega\,(1-\omega^2)^{-1/2}\ln[1+\sqrt{2}\,\omega(1+\omega^2)^{-1/2}] . \tag{2.33}$$

The integral in (2.30) may be written as

$$I_3 - \pi^{-1}n^{-1}\Sigma_2(\tau n^{-1}, \sigma^2 n^{-1}) = \pi^{-1}n^{-1}\int_{1/n}^{1} d\omega \ln[1+(\sigma^2+\tau)(\tau^2+n^2\omega^2)^{-1/2}] - \pi^{-1}n^{-2}\int_1^c d\xi \ln[1+(\tau+\sigma^2)(\tau^2+\xi^2)^{-1/2}] . \tag{2.34}$$

On integrating by parts, the first integral becomes

$$\int_{1/n}^{1} d\omega \ln[1+(\sigma^2+\tau)(\tau^2+n^2\omega^2)^{-1/2}] = \{\omega \ln[1+(\sigma^2+\tau)(\tau^2+n^2\omega^2)^{-1/2}]\}_{1/n}^{1} - \int_{1/n}^{1} d\omega\,\omega\frac{d}{d\omega}\{\ln[1+(\sigma^2+\tau)(\tau^2+n^2\omega^2)^{-1/2}]\} . \tag{2.35}$$

The second term in this equation is an integral over a rational function $R(\omega^2, X)$, where $X=(\tau^2+n^2\omega^2)^{1/2}$. It can then be broken up by partial fractions into terms of the types

$$\int d\omega X^{-1}, \quad \int d\omega X^{-1}(a^2+\omega^2)^{-1}, \quad \int d\omega\,(a^2+\omega^2)^{-1} . \tag{2.36}$$

These elementary integrals can be evaluated,[19] and (2.35) become

$$\int_{1/n}^{1} d\omega \ln[1+(\sigma^2+\tau)(\tau^2+n^2\omega^2)^{-1/2}] \approx (\tau+\sigma^2)n^{-1}\ln n + Q(\tau,\sigma^2) , \tag{2.37}$$

in which

$$Q(\tau,\sigma^2) = (\tau+\sigma^2) - \ln[1+(\tau+\sigma^2)(1+\tau^2)^{-1/2}] + (\tau+\sigma^2)\{\ln 2 - \ln[1+(\tau^2+1)^{1/2}]\} + \tau[\tan^{-1}(1/\tau) - \mathrm{sgn}(\tau)\pi/2] - \sigma(\sigma^2+2\tau)^{1/2}\mathfrak{L}(\tau,\sigma^2) , \tag{2.38}$$

where $\mathfrak{L}(\tau,\sigma^2)$ is the function defined by (1.23). Consequently, Eq. (2.34) becomes

$$I_3 = -\pi^{-1}n^{-2}\int_1^c d\xi \ln[1+(\sigma^2+\tau)(\tau^2+\xi^2)^{-1/2}] + \pi^{-1}(\tau+\sigma^2)n^{-2}\ln n + \pi^{-1}n^{-2}Q(\tau,\sigma^2) + n^{-1}D_1 + n^{-2}(\tau+\sigma^2)D_3 + E_3 + O(n^{-5/2}) . \tag{2.39}$$

Finally, we turn to the integral I_2 given by (2.17). Note that the integration is from the origin to $c/n = n^{-1/2}$, and $n^{-1/2} \ll 1$. In this interval, one can write

$$v_\pm = 1 \pm \tau(\tau^2+\xi^2)^{-1/2} + O(n^{-1}) , \tag{2.40}$$

$$e^{-n\xi} = e^{-4(\tau^2+\xi^2)^{1/2}}[1+O(n^{-1})] , \tag{2.41}$$

$$u = \sigma^2(\tau^2+\xi^2)^{-1/2} + O(n^{-1}) , \tag{2.42}$$

and

$$(1-\omega^2)^{-1/2}=1+O(n^{-1}) \ . \tag{2.43}$$

Hence

$$I_2=\pi^{-1}n^{-2}\int_0^c d\xi \ln\left[1+\frac{\tau+\sigma^2}{(\tau^2+\xi^2)^{1/2}}+\left(1-\frac{\tau+\sigma^2}{(\tau^2+\xi^2)^{1/2}}\right)e^{-4(\tau^2+\xi^2)^{1/2}}\right]+E_2 \ . \tag{2.44}$$

The sum of the correction terms E_2 and E_3 is shown, in Appendix D, to be of the order $n^{-5/2}$. Let us make the abbreviations

$$X(\xi)=(\tau^2+\xi^2)^{1/2} \ , \tag{2.45}$$

$$p(\xi)=1+(\tau+\sigma^2)/X(\xi) \ , \tag{2.46}$$

and

$$q(\xi)=1-(\tau+\sigma^2)/X(\xi) \ , \tag{2.47}$$

so that we may write (2.37) as

$$I_2\approx\pi^{-1}n^{-2}\int_0^1 d\xi \ln[p(\xi)+q(\xi)e^{-4X(\xi)}]+\pi^{-1}n^{-2}\int_1^c d\xi\ln[p(\xi)+q(\xi)e^{-4X(\xi)}] \ . \tag{2.48}$$

Now consider the sum of the integrals in (2.28), (2.39), and (2.48), namely,

$$\begin{aligned}\tilde{R}(\tau,\sigma^2)&=\int_0^1 d\xi\, 2X(\xi)-\int_1^c d\xi\,\ln[p(\xi)]+\int_0^1 d\xi\,\ln[p(\xi)+q(\xi)e^{-4X(\xi)}]+\int_1^c d\xi\,\ln[p(\xi)+q(\xi)e^{-4X(\xi)}] \ ,\\ &=\int_0^1 d\xi\,\ln[p(\xi)e^{2X(\xi)}+q(\xi)e^{-2X(\xi)}]+\int_1^c d\xi\,\ln[1+q(\xi)p^{-1}(\xi)e^{-4X(\xi)}] \ .\end{aligned} \tag{2.49}$$

On expanding $\ln(1+p^{-1}q\,e^{-4X})$ in powers of e^{-4X}, one sees that

$$\int_c^\infty d\xi\,\ln(1+p^{-1}q\,e^{-4X})=O(e^{-4c}), \tag{2.50}$$

so that we find

$$\tilde{R}(\tau,\sigma^2)\approx R(\tau,\sigma^2)=\int_0^1 d\xi\,\ln(p\,e^{2X}+q\,e^{-2X})+\int_1^\infty d\xi\,\ln(1+p^{-1}q\,e^{-4X}). \tag{2.51}$$

On combining (2.28), (2.39), and (2.48), and using (2.51), we get finally,

$$\begin{aligned}\Delta f(n,t,h_1)=I_1+I_2+I_3&=2G/\pi+n^{-1}D_1+(\tau^2+\tau+\sigma^2)\pi^{-1}n^{-2}\ln n+n^{-2}\pi^{-1}[R(\tau,\sigma^2)+Q(\tau,\sigma^2)+P(\tau)\\ &+\tfrac{1}{2}\tau^2\ln 2+(\tau+\sigma^2)(\tfrac{1}{2}\ln 2+\pi/4-\tfrac{1}{2}\pi\sqrt{2})]+O(n^{-5/2}) \ .\end{aligned} \tag{2.52}$$

The functions $R(\tau,\sigma^2)$, $Q(\tau,\sigma^2)$, and $P(\tau)$ are given by (2.51), (2.38), and (2.27), respectively. If we define

$$Y(\tau,\sigma^2)=[R(\tau,\sigma^2)+Q(\tau,\sigma^2)+P(\tau)+\tfrac{1}{2}\tau^2\ln 2+(\tau+\sigma^2)(\tfrac{1}{2}\ln 2+\pi/4-\pi\sqrt{2})]/\pi, \tag{2.53}$$

then the free energy is indeed in the form quoted in the Introduction.

At the critical temperature in zero field ($T=T_c$, $H_1=0$), we have

$$R(0,0)=2\int_0^1 d\xi\,\xi+\int_0^\infty d\xi\,\ln(1+e^{-4\xi})=1+\pi^2/48 \ , \tag{2.54}$$

$$Q(0,0)=0 \ , \tag{2.55}$$

$$P(0)=-1 \ , \tag{2.56}$$

and

$$\ln\cosh K_c=\tfrac{1}{2}\ln(1+\sqrt{2})-\tfrac{1}{2}\ln 2 \ . \tag{2.57}$$

Hence the free energy (2.1) at the critical point is

$$f(n,0,0)=f_c(n)\approx\tfrac{1}{2}\ln 2+2G/\pi+n^{-1}[D_1-\tfrac{1}{2}\ln(1+\sqrt{2})]+n^{-2}(\pi/48), \tag{2.58}$$

where D_1 was defined in (1.29). The reduced energy per spin is given explicitly by

$$u(n,t,h_1)\approx-n\left(\frac{\partial f}{\partial t}\right)_\sigma\approx\tfrac{1}{2}\coth 2K-\tfrac{1}{2}n^{-1}\tanh K-(\pi n)^{-1}(2\tau+1)\ln n-(n\pi)^{-1}\Big[\tfrac{1}{2}\ln 2+\pi/4-\tfrac{1}{2}\pi\sqrt{2}+\tau\ln 2$$

$$+(2\tau+1)\{\ln 2-\ln[1+(\tau^2+1)^{1/2}]\}+\tan^{-1}(1/\tau)-\mathrm{sgn}(\tau)\pi/2-\sigma(\sigma^2+2\tau)^{-1/2}\mathfrak{L}(\tau,\sigma^2)+\left(\frac{\partial R}{\partial\tau}\right)_\sigma\Bigg]. \tag{2.59}$$

At the critical point, itself, we have

$$\frac{\partial}{\partial\tau}R(0,0)=\int_0^1 d\xi\,\xi^{-1}\tanh 2\xi-2\int_1^\infty d\xi\,\xi^{-1}(e^{4\xi}+1)^{-1}\equiv\gamma+3\ln 2-\ln\pi, \tag{2.60}$$

and so

$$u(n,0,0)=u_c(n)\approx\tfrac12\sqrt2-(\pi n)^{-1}\ln n-(n\pi)^{-1}(-\pi/4+\tfrac72\ln 2+\gamma-\ln\pi). \tag{2.61}$$

The specific heat can be written as

$$\begin{aligned}C(n,t,h_1)\approx{}&A_0\ln n+A_0\{\ln 2-\ln[1+(\tau^2+1)^{1/2}]\}+\tfrac12A_0(\ln 2-\pi/2)-\tfrac12A_0(1+\tau^2)^{-1}-A_0\tau^2[(\tau^2+1)^{1/2}+1+\tau^2]^{-1}\\&\times[1+(\sigma^2+2\tau)^{-1}]-\tfrac12A_0\sigma^2(\sigma^2+2\tau)^{-1}[\tau^2+1+(\sigma^2+\tau)(\tau^2+1)^{1/2}]\\&+\tfrac12A_0\sigma(\sigma^2+2\tau)^{-3/2}\mathfrak{L}(\tau,\sigma^2)+\tfrac12A_0\left(\frac{\partial^2R(\tau,\sigma^2)}{\partial\tau^2}\right)_{\sigma^2=0},\end{aligned} \tag{2.62}$$

where A_0 was defined in (1.33) and the corrections are of order $n^{-1/2}$ or smaller. At the critical temperature in zero field, we have

$$\begin{aligned}\frac{\partial^2R(0,0)}{\partial\tau^2}&=2\int_0^1 d\xi\,\xi^{-1}\tanh 2\xi-4\int_1^\infty d\xi\,\xi^{-1}(e^{4\xi}+1)^{-1}-\int_0^1 d\xi\,\xi^{-2}\tanh^2 2\xi+2\int_1^\infty d\xi\,\xi^{-2}(e^{4\xi}+1)^{-2}\\&=2(\gamma+3\ln 2-\ln\pi)+1-28\zeta(3)/\pi^2\end{aligned} \tag{2.63}$$

and

$$C(n,0,0)=C_c(n)=A_0\ln n+A_0[\gamma+\tfrac72\ln 2-\ln\pi-14\zeta(3)/\pi^2-\pi/4], \tag{2.64}$$

where $\zeta(3)\simeq 1.2020569$ is the Riemann ζ function and $\gamma\simeq 0.5772157$ is the Euler's constant.

We define the boundary or surface layer magnetization by

$$\begin{aligned}M_1(n,t,h_1)=n\left(\frac{\partial f}{\partial h_1}\right)\approx h_1+2(1+\sqrt2)\pi^{-1}h_1\Bigg(&\ln n+\ln 2-\ln[1+(\tau^2+1)^{1/2}]-(\sigma^2+\tau)\sigma^{-1}(\sigma^2+2\tau)^{-1/2}\mathfrak{L}(\tau,\sigma^2)\\&+\tfrac12\ln 2+\pi/4-\tfrac12\pi\sqrt2+\frac{\partial R(\tau,\sigma^2)}{\partial\sigma^2}\Bigg).\end{aligned} \tag{2.65}$$

We find from the above expression that the *spontaneous* boundary magnetization $M_1(n,t,0)$ vanishes identically for all t (as expected for $n<\infty$).

The boundary susceptibility is likewise given by

$$\begin{aligned}\chi_{11}(n,t,h_1)=\frac{\partial M_1(n,t,h_1)}{\partial h_1}\approx 1+2(1+\sqrt2)\pi^{-1}\Bigg[&\ln n+\ln 2-\ln[1+(\tau^2+1)^{1/2}]-(\sigma^2+\tau)\sigma^{-1}(\sigma^2+2\tau)^{-1/2}\mathfrak{L}(\tau,\sigma^2)\\&+\tfrac12\ln 2+\pi/4-\tfrac12\pi\sqrt2-2(\sigma^2+\tau)(\sigma^2+2\tau)^{-1}\{1-[(1+\tau^2)^{1/2}+\tau+\sigma^2]^{-1}\}\\&+2\tau^2(\sigma^2+2\tau)^{-3/2}\sigma^{-1}\mathfrak{L}(\tau,\sigma^2)+\frac{\partial R(\tau,\sigma^2)}{\partial\sigma^2}+2\sigma^2\left(\frac{\partial^2R(\tau,\sigma^2)}{\partial(\sigma^2)^2}\right)\Bigg].\end{aligned} \tag{2.66}$$

In particular, at the critical point $T=T_c$, $h_1=0$, we have

$$\chi_{11}(n,0,0)\approx 2(1+\sqrt2)\pi^{-1}\ln n+2(1+\sqrt2)\pi^{-1}(\gamma+\tfrac72\ln 2-\ln\pi)-\tfrac12(\sqrt2+1). \tag{2.67}$$

III. PROPERTIES OF THE SCALING FUNCTION

We shall first show that the scaling function $Y(\tau,\sigma^2)$ of (1.22) is analytic. It is obvious from (1.22) that the only possible singularity of $Y(\tau,\sigma^2)$ can come from the function $\mathfrak{L}(\tau,\sigma^2)$ and the integral $R(\tau,\sigma^2)$. We differentiate $\mathfrak{L}(\tau,\sigma^2)$ with respect to τ, and find

$$\frac{\partial\mathfrak{L}(\tau,\sigma^2)}{\partial\tau}=\sigma(\sigma^2+2\tau)^{-1/2}\{\tau^{-1}[(\tau^2+1)^{1/2}-1]$$

$$+[(\tau^2+1)^{1/2}(\sigma^2+\tau)+(\tau^2+1)]^{-1}\}, \tag{3.1}$$

and with respect to σ^2, to obtain

$$\frac{\partial\mathfrak{L}(\tau,\sigma^2)}{\partial\sigma^2}=\sigma^{-1}(\sigma^2+2\tau)^{-1/2}\{1-[(\tau^2+1)^{1/2}+\sigma^2+\tau]^{-1}\}. \tag{3.2}$$

Using these relations and the fact that $\mathfrak{L}(\tau,\sigma^2)$ is odd in $(\sigma^2+2\tau)^{1/2}$, one can show that the derivatives of $\sigma(\sigma^2+2\tau)^{1/2}\mathfrak{L}(\tau,\sigma^2)$ with respect to τ and to σ^2 are analytic functions in τ and σ^2. Hence $\sigma(\sigma^2+2\tau)^{1/2}\mathfrak{L}(\tau,\sigma^2)$, itself, must also be analytic. The function $R(\tau,\sigma^2)$, given by (1.24), is a sum of two integrals, whose integrands contain the term $X(\xi)=(\tau^2+\xi^2)^{1/2}$ which has branch points at $\xi=\pm i\tau$. However, as the integration in the second integral runs from 1 to ∞, one concludes that it is analytic for all real τ and σ^2. As for the integrand of the first integral, one can see that it is analytic in $X=X(\xi)$. Moreover, since $(e^{2X}+e^{-2X})$ and $(e^{2X}-e^{-2X})/X$ are even functions of X, one finds that the integrand has a convergent Taylor expansion in $X^2=(\tau^2+\xi^2)$. This shows that the first integral is also analytic in τ and σ^2. Hence, we have shown that the scaling function is analytic, as expected on general grounds.

When $\tau\sim n/\xi\sim nt\gg 1$, we rewrite (2.30) and (2.44) in the form

$$I_2+I_3=(n\pi)^{-1}\int_0^1 d\omega\,\ln[1+(\sigma^2+\tau)(\tau^2+n^2w^2)^{-1/2}] + (n\pi)^{-1}\Sigma_2(\tau/n,\sigma^2/n)+n^{-2}e(\tau,\sigma^2), \quad (3.3)$$

where $e(\tau,\sigma^2)$ is the correction term,

$$e(\tau,\sigma^2)=\pi^{-1}\int_0^\infty d\xi\,\ln[1+p^{-1}(\xi)q(\xi)\,e^{-4X(\xi)}]\,. \quad (3.4)$$

Since $X(\xi)=(\tau^2+\xi^2)^{1/2}$ and $e^{-4X}\leqslant e^{-4\tau}$, one expects the term $e(\tau,\sigma^2)$ to be exponentially small in τ. The detailed analysis of $e(\tau,\sigma^2)$ is described in Sec. IV.

Consequently, the free energy Δf of (2.15) can be written as

$$\Delta f=I_1+I_2+I_3 =\Delta f^\infty(t)+n^{-1}[\Delta f^\times(t,0_1)+\Delta f^\times(t,h_1)]+n^{-2}e(\tau,\sigma^2) \quad (3.5)$$

where the bulk free energy is given by

$$\Delta f^\infty(t)=I_1\,, \quad (3.6)$$

and the boundary free energy by

$$\Delta f^\times(t,0)+\Delta f^\times(t,h_1)=n(I_2+I_3)-n^{-1}e(\tau,\sigma^2)\,. \quad (3.7)$$

By (2.10) and (3.6), one finds that the bulk free energy can be written explicitly as

$$\Delta f^\infty(t)=\pi^{-1}\int_0^1 2(\tau^2n^{-2}+\omega^2)^{1/2}+\Sigma_1(\tau n^{-1})\approx 2G/\pi+\pi^{-1}(1+\ln 2)2K_c^2t^2-\pi^{-1}4K_c^2t^2\ln|K_ct|\,. \quad (3.8)$$

Thus the bulk specific heat diverges as $C^\infty(t)\approx-(8K_c^2/\pi)\ln|t|$. This is identical to Onsager's result.[1]

The boundary free energy $\Delta f^\times(t,h_1)$, given by (3.7) and (3.3), is an integral:

$$\Delta f^\times(t_1,0)+\Delta f^\times(t,h_1)=\pi^{-1}\int_0^1 d\omega\,\ln[1+(\sigma^2+\tau)(\tau^2+n^2\omega^2)^{-1/2}]+\pi^{-1}\Sigma_2(\tau n^{-1},\sigma^2n^{-1})\,. \quad (3.9)$$

This integral is identical to that in Eq. (2.37), except that the lower limit of integration is changed from n^{-1} to zero. Hence it can be evaluated in closed form, and we find

$$\Delta f^\times(t_1,0)+\Delta f^\times(t_1,h_1)\approx\pi^{-1}2K_ct\ln|K_ct|^{-1}X_1^\times(\sigma/\tau^{1/2})+\pi^{-1}2K_ctX_2^\times(\sigma/\tau^{1/2})+D_1\,, \quad (3.10)$$

where D_1 is given in (1.29), while

$$X_1^\times(y)=1+y^2 \quad (3.11)$$

and

$$X_2^\times(y)=(1+\tfrac12\ln 2+\pi/4-\tfrac12\pi\sqrt2)(1+y^2)-\tfrac12\pi\,\mathrm{sgn}(\tau)+\pi\,|y(-2-y^2)^{1/2}|\,\Theta(-y^2)\Theta(1+y^2) -\tfrac12y(y^2+2)^{1/2}\{\ln[1+y^2+y(y^2+2)^{1/2}]-\ln[1+y^2-y(y^2+2)^{1/2}]\}\,. \quad (3.12)$$

Note that $y^2=\sigma^2/\tau$ may be positive or negative. In (3.12), $\Theta(x)$ is the Heaviside function defined by

$$\Theta(x)=\begin{cases}1 & \text{for } x>0\,,\\ 0 & \text{for } x<0\,.\end{cases} \quad (3.13)$$

When the boundary field vanishes ($\sigma^2=y^2=0$), one finds

$$X_1^\times(0)=1 \quad\text{and}\quad X_2^\times(0)=1+\tfrac12\ln 2+\pi/4-\tfrac12\pi\sqrt2-\tfrac12\pi\,\mathrm{sgn}(\tau)\,. \quad (3.14)$$

Hence, the boundary free energy in zero field can be written as

$$2f^\times(\tau,0)=2\Delta f^\times(t,0)+2f_0^\times(t,0) =\pi^{-1}2K_ct\ln|K_ct|^{-1} +2K_ct[\pi^{-1}+\pi^{-1}\tfrac12\ln 2+\tfrac14-\tfrac12\sqrt2-\tfrac12\mathrm{sgn}(\tau)] -\cosh K-\tfrac12\ln 2+D_1\,. \quad (3.15)$$

At the critical temperature ($T=T_c$), the boundary free energy of a semi-infinite lattice is given by

$$2f^\times(T_c, 0) = D_1 - \tfrac{1}{2}\ln(1+\sqrt{2})\ . \tag{3.16}$$

This is identical to the result found by Ferdinand and Fisher.[2] It is obvious from (3.15) that the derivative of $f^\times(T,0)$ with respect to temperature not only has a logarithmic singularity at T_c, but also has a superimposed discontinuity there.[13] The boundary specific heat, which is proportional to the second derivative of $f^\times(T,0)$ with respect to T, diverges linearly as

$$C^\times(T) \approx -\pi^{-1}K_c t^{-1}\ . \tag{3.17}$$

This is identical to the results of McCoy and Wu,[13] and of Ferdinand and Fisher.[2]

In the limit $y^2 = \sigma^2/\tau \propto h_1^2/t \to \infty$, we find from (3.1) and (3.12) that

$$V_1(0) = \lim_{y\to\infty} y^{-2}X_1^\times(y) = 1 \tag{3.18}$$

and

$$V_2(0) = \lim_{y\to\infty}[2y^{-2}\ln|y|X_1^\times(y) + y^{-2}X_2^\times(y)]$$
$$= 1 + \tfrac{1}{2}\ln 2 + \pi/4 - \tfrac{1}{2}\pi\sqrt{2}\ . \tag{3.19}$$

This agrees with the scaling prediction of (1.15) and (1.16). For small y^{-1} we can write

$$V_1(v) = v^2X_1^\times(v^{-1}) = 1 + v^2 \quad \text{with } v = y^{-1}\ , \tag{3.20}$$

and

$$V_2(v) = 2v^2\ln|v|^{-1}X_1^\times(v^{-1}) + v^2X_2^\times(v^{-1})$$
$$= (1 - \tfrac{1}{2}\ln 2 + \pi/4 - \tfrac{1}{2}\pi\sqrt{2}) - v^2[\tfrac{1}{2}\ln 2 + \pi/4 - \tfrac{1}{2}\pi\sqrt{2}]$$
$$- \tfrac{1}{2}\pi|v^2| - \tfrac{1}{2}v^4\ln v^2 + O(v^4)\ . \tag{3.21}$$

Hence the boundary free energy of (3.10) can be written as

$$\Delta f^\times(t,0) + \Delta f^\times(t,h_1) \approx D_1 + \pi^{-1}(1+\sqrt{2})z^2$$
$$\times\{-\ln z^2 - \ln(1+\sqrt{2}) + 1 + \tfrac{1}{2}\ln 2$$
$$+ \pi/4 - \tfrac{1}{2}\pi\sqrt{2}\} + O(t)\ . \tag{3.22}$$

The boundary or surface layer magnetization[13] of a semi-infinite lattice behaves at T_c as

$$M_1^\times(T_c, h_1) = \frac{\partial}{\partial h_1} f^\times(t,h_1)\bigg|_{t=0}$$
$$\approx -\pi^{-1}4(1+\sqrt{2})z\ln z \approx -\pi^{-1}4(1+\sqrt{2})h_1\ln h_1\ . \tag{3.23}$$

In the other limit, when h_1 is small but nonzero, such that $\sigma^2/2\tau \sim h_1^2/2t \ll 1$, Eq. (3.10) yields

$$\Delta f^\times(t,h_1) \approx 2(1+\sqrt{2})^{1/2}(K_c|t|)^{1/2}\Theta(-t)z - \pi^{-1}$$
$$-\pi^{-1}(1+\sqrt{2})z^2\ln|K_c t| + [\pi^{-1}(\tfrac{1}{2}\ln 2 - 1) + \tfrac{1}{4} - \tfrac{1}{2}\sqrt{2}]z^2 \tag{3.24}$$

This then gives the surface-layer spontaneous magnetization of a semiinfinite Ising model, namely,

$$M_1^\times(t,0) = \lim_{h_1\to 0}\frac{\partial}{\partial h_1}[f^\times(t_1h_1)]$$
$$= 2(1+\sqrt{2})^{1/2}K_c^{1/2}|t|^{1/2}\Theta(-t)\ , \tag{3.25}$$

while the boundary susceptibility behaves as

$$\chi_{11}^\times(t,0) = \lim\frac{\partial}{\partial h_1}M_1^\times(t,h_1)$$
$$\approx -2(1+\sqrt{2})\pi^{-1}\ln|t|\ . \tag{3.26}$$

These results agree with the computation by McCoy and Wu.[13]

IV. CORRECTIONS TO THE BULK-PLUS-SURFACE BEHAVIOR

In this section, we consider the correction term

$$e(\tau,\sigma^2) = \pi^{-1}\int_0^\infty d\xi\ln[1 + p^{-1}(\xi)q(\xi)e^{-4X(\xi)}] \tag{4.1}$$

to the bulk and surface behavior for large τ. In (4.1), we have

$$p(\xi) = 1 + (\tau+\sigma^2)/X(\xi) \tag{4.2}$$

and

$$q(\xi) = 1 - (\tau+\sigma^2)/X(\xi)\ . \tag{4.3}$$

For large τ, one may write

$$e^{-4X(\xi)} = e^{-4|\tau|}e^{-2\xi^2/|\tau|}[1 + O(\xi^4/|\tau|^3)] \tag{4.4}$$

and

$$(\tau+\sigma^2)/X(\xi) = [\mathrm{sgn}(\tau) + \sigma^2/|\tau|]$$
$$-\tfrac{1}{2}\xi^2\tau^{-2}[\mathrm{sgn}(\tau) + \sigma^2/|\tau|] + O(\xi^4/|\tau|^4)\ . \tag{4.5}$$

When $T > T_c$ $(\tau > 0)$, it is obvious from (4.2) that $p(\xi) \geq 1$. Hence, $p^{-1}q e^{-4X}$ is small for large τ. On expanding the logarithm in powers of $p^{-1}q e^{-4X}$, one finds

$$e(\tau,\sigma^2) = \pi^{-1}\int_0^\infty d\xi\, p^{-1}q\, e^{-4X(\xi)} + O(e^{-8\tau}) \quad \text{for} \quad T > T_c\ . \tag{4.6}$$

We may substitute (4.2)–(4.5) into this equation to get

$$e(\tau,\sigma^2) = \pi^{-1}e^{-4|\tau|}$$
$$\times\int_0^\infty d\xi\left[\frac{-\sigma^2/\tau}{2+\sigma^2/\tau} + \frac{1+\sigma^2/\tau}{(2+\sigma^2/\tau)^2}\xi^2\tau^{-2}\right]e^{-2\xi^2/|\tau|}\ . \tag{4.7}$$

These Gaussian integrals can be evaluated easily, and we find

$$e(\tau,\sigma^2) \approx e^{-4|\tau|}E^+(\tau,\sigma^2/\tau)\ , \tag{4.8}$$

in which

$$E^+(\tau,y^2) = (8\pi)^{-1/2}[\tau^{1/2}(-y^2)(2+y^2)^{-1}$$
$$+ \tau^{-1/2}(1+y^2)4^{-1}(2+y^2)^{-2}]\ . \tag{4.9}$$

When the external field h_1 vanishes $(y=0)$, we have

$$E^+(\tau, 0) = E_0^+(\tau) = (32)^{-1}(2\pi\tau)^{-1/2}, \tag{4.10}$$

and the leading correction term is simply

$$e(\tau, 0) \approx (32)^{-1}(2\pi\tau)^{-1/2} e^{-4\tau}. \tag{4.11}$$

When the field is nonzero ($y \neq 0$), we find from (4.9) that

$$E^+(\tau, y^2) \approx (8\pi)^{-1/2}(-y^2)(2+y^2)^{-1}\tau^{1/2}[1+O(\tau^{-1})]. \tag{4.12}$$

Hence, the leading term of the function $e(\tau, \sigma^2)$ for large τ is

$$e(\tau, \sigma^2) \approx (8\pi)^{-1/2}(-y^2)(2+y^2)^{-1}\tau^{1/2} e^{-4\tau}. \tag{4.13}$$

When the temperature is below T_c ($\tau < 0$), one finds from (4.2) that

$$p(\xi) = \sigma^2/|\tau| + \tfrac{1}{2}\xi^2\tau^{-2}(1+\sigma^2/\tau) + O(\xi^4\tau^{-4}). \tag{4.14}$$

Therefore $p(\xi)^{-1}$ can be very large when ξ and $\sigma^2/|\tau|$ are sufficiently small. For this reason, we may not use the expansion of the logarithm, as we did for $T > T_c$. We integrate (4.1) by parts, and find

$$e(\tau, \sigma^2) = \pi^{-1}\int_0^\infty d\xi \frac{\xi^2}{X}\frac{4q^2 e^{-4X}}{p+q e^{-4X}} - \pi^{-1}\int_0^\infty d\xi \frac{\xi^2\tau}{X^3}\frac{2(1+\sigma^2/\tau)e^{-4X}}{p(p+qe^{-4X})}. \tag{4.15}$$

When τ is large, we may make the following approximations:

$$p + q e^{-4X} \approx \sigma^2/|\tau| + \tfrac{1}{2}\xi^2\tau^{-2}(1+\sigma^2/\tau) + (2+\sigma^2/\tau)e^{-4|\tau|}, \tag{4.16}$$

$$p \approx \sigma^2/|\tau| + \tfrac{1}{2}\xi^2\tau^{-1/2}(1+\sigma^2/\tau), \tag{4.17}$$

$$q \approx (2+\sigma^2/\tau) - \tfrac{1}{2}\xi^2\tau^{-2}(1+\sigma^2/\tau), \tag{4.18}$$

and

$$\xi^2/X \approx \xi^2/|\tau|, \quad \xi^2\tau/X^3 \approx -\xi^2/\tau^2. \tag{4.19}$$

Substituting (4.16)–(4.19) into (4.15), and then neglecting the term of the order $e^{-8|\tau|}$, we find

$$\begin{aligned} e(\tau, \sigma^2) \approx\ & 4(e^{-4|\tau|}/\pi|\tau|)\int_0^\infty [2x^{-2} - \xi^2 - 2y^2x^{-2}(y^2+\delta^2+\xi^2x^2)^{-1}]e^{-2\xi^2/|\tau|}d\xi, \\ & + 4(e^{-4|\tau|}/\pi)\int_0^\infty (y^2+\delta^2+\xi^2x^2)^{-1}e^{-2\xi^2/|\tau|}d\xi, \\ & + 4(e^{-4|\tau|}y^2/\pi\delta^2)\int_0^\infty [(y^2+\delta^2+\xi^2x^2)^{-1} - (y^2+\xi^2x^2)^{-1}]e^{-2\xi^2/|\tau|}d\xi, \end{aligned} \tag{4.20}$$

where we have written

$$y^2 = \sigma^2/|\tau|, \tag{4.21}$$

$$x^2 = \tfrac{1}{2}\tau^{-2}(1-y^2), \tag{4.22}$$

and

$$\delta^2 = (2-y^2)e^{-4|\tau|}. \tag{4.23}$$

Let us define a function

$$\Phi(\lambda) = \int_0^\infty \frac{e^{-\lambda u^2}}{1+u^2}du. \tag{4.24}$$

It is easy to show that

$$\Phi(0) = \pi/2, \tag{4.25}$$

$$\Phi(\lambda) = \Phi(0) + O(\lambda^{1/2}) \quad \text{as} \quad \lambda \to 0, \tag{4.26}$$

$$\Phi(\lambda) = \tfrac{1}{2}(\pi/\lambda)^{1/2} + O(\lambda^{-3/2}) \quad \text{as} \quad \lambda \to \infty. \tag{4.27}$$

Now, the integrals in (4.20) can be written in terms of the function Φ yielding the final result

$$\begin{aligned} e(\tau, \sigma^2) \approx\ & 4e^{-4|\tau|}(2\pi|\tau|)^{-1/2}(x^{-2} - |\tau|/8) - 8e^{-4|\tau|}y^2\pi^{-1}x^{-3}(y^2+\delta^2)^{-1/2}\Phi(2(y^2+\delta^2)/|\tau|x^2) \\ & + 4e^{-4|\tau|}\pi^{-1}x^{-1}(y^2+\delta^2)^{-1/2}\Phi(2(y^2+\delta^2)/|\tau|x^2) + 4e^{-4|\tau|}\pi^{-1}y^2x^{-1} \\ & \times\delta^{-2}[(y^2+\delta^2)^{-1/2}\Phi(2(y^2+\delta^2)/|\tau|x^2) - |y|^{-1}\Phi(2y^2/|\tau|x^2)]. \end{aligned} \tag{4.28}$$

When the field is zero ($h_1 = \sigma = y = 0$), we have

$$\Phi(2\delta^2/|\tau|x^2) = \pi/2 + O(\delta). \tag{4.29}$$

Hence (4.28) becomes

$$e(\tau, 0) \approx 2|\tau|e^{-2|\tau|} + O(e^{-4|\tau|}). \tag{4.30}$$

When the field is nonvanishing, we find $\delta^2 \sim e^{-4|\tau|} \ll y^2$ for large τ, and we can make the Taylor expansions

$$(y^2+\delta^2)^{-1/2} = |y|^{-1} - \tfrac{1}{2}\delta^2|y|^{-3} + O(\delta^4), \tag{4.31}$$

$$\begin{aligned}\Phi(2(y^2+\delta^2)|\tau|^{-1}x^{-2}) =\ & \Phi(2y^2|\tau|^{-1}x^{-2}) + 2\delta^2|\tau|^{-1}x^{-2} \\ & \times[\Phi(2y^2|\tau|^{-1}x^{-2}) - \tfrac{1}{2}(\pi|\tau|/2)^{1/2}xy^{-1}] + O(\delta^4).\end{aligned} \tag{4.32}$$

In (4.32), we have used the identity

$$\frac{\partial}{\partial\lambda}\Phi(\lambda) = \Phi(\lambda) - \tfrac{1}{2}(\pi/\lambda)^{1/2}. \tag{4.33}$$

Substituting (4.31) and (4.32) into (4.28), we get

$$e(\tau,\sigma^2)\approx e^{-4|\tau|}E^{-1}(\tau,\sigma^2)\ , \tag{4.34}$$

where

$$E^{-}(\tau,\sigma^2) = -(8\pi)^{-1/2}|\tau|^{1/2}+2\pi^{-1}x^{-1}y^{-1}\Phi(2y^2|\tau|^{-1}x^2)\,. \tag{4.35}$$

When $y^2>\frac{1}{2}$, the argument of the function Φ is large, that is,

$$2y^2|\tau|^{-1}x^2 = 4|\tau|y^2(1-y^2)^{-1}\gg 1\ , \tag{4.36}$$

so that on using (4.29), we find

$$E^{-}(\tau,\sigma^2)\approx -(8\pi)^{-1/2}|\tau|^{1/2}(y^2-2)y^{-2} \quad \text{for} \quad y^2>\tfrac{1}{2}\ . \tag{4.37}$$

In the limit $h_1\sim y\to 0$, the second term in (4.35) diverges, so that the more complete expression (4.28) must be used and (4.30) results.

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APPENDIX A: COMPARISON OF NOTATION

In this article, we use the notation

$$\lambda_+(\omega) = z_1^{-1}(1-z_1^2)^{-1}|1+z_1e^{i\theta}|^2\lambda(\theta) \tag{A1}$$

and

$$\lambda_-(\omega) = z_1^{-1}(1-z_1^2)^{-1}|1+z_1e^{i\theta}|^2\lambda'(\theta)\ , \tag{A2}$$

in which the variable ω is defined by

$$\omega = \sin(\theta/2)\ , \tag{A3}$$

and the functions $\lambda_\pm(\omega)$ are defined in (2.4), and $\lambda(\theta)$ and $\lambda'(\theta)$ are given[13] by Eq. (3.14) in McCoy and Wu's paper. We also write

$$v_+(\omega) = 2v^2(\theta)\ , \tag{A4}$$

$$v_-(\omega) = 2v'^2(\theta)\ , \tag{A5}$$

and

$$u(\omega) = -2v(iv')z_2^{-1}c^{-1}\ , \tag{A6}$$

with

$$c = 2i\sin\theta\,|1+e^{i\theta}|^{-2}\ , \tag{A7}$$

where $v_\pm(\omega)$, and $u(\omega)$ are defined in (2.5) and (2.6), while $v(\theta)$ and $v'(\theta)$ are given by Eq. (3.19) in Ref. 13.

APPENDIX B: THE CORRECTION TERM E_1

The correction term E_1 defined in (2.19) can be written as

$$E_1 = (\pi n)^{-1}\int_{c/n}^{1} d\omega(1-\omega^2)^{-1/2}\ln[1+\chi(\omega)e^{-n\xi}]\ , \tag{B1}$$

where

$$\chi(\omega) = (v_- - z^2u)(v_+ + z^2u)^{-1}\ . \tag{B2}$$

Since $z^2u(\omega)$ is nonnegative for all ω and τ, one finds

$$|\chi(\omega)|\le|v_-/v_+|\ . \tag{B3}$$

Furthermore, one can readily establish the inequality

$$\tfrac{1}{2}(v_+ - v_-)\ge -|\tau|(\tau^2+n^2\omega^2)^{-1/2}\ . \tag{B4}$$

Combination of Eqs. (B3) and (B4) yields

$$|\chi(\omega)|\le 4+\tau^2c^{-2}\ . \tag{B5}$$

Because $\chi(\omega)$ is bounded, we can expand the logarithm in (B1) to find

$$E_1 = (\pi n)^{-1}\int_{c/n}^{1} d\omega(1-\omega^2)^{-1/2}\chi(\omega)e^{-n\xi}+O(e^{-2n\xi})\ . \tag{B6}$$

From (2.14) and (B5), we find that

$$E_1\le(2n)^{-1}(4+\tau^2c^{-2})e^{-4c}+O(e^{-8c})\ , \tag{B7}$$

so that E_1 is of the order e^{-4c}.

APPENDIX C: ASYMPTOTIC EXPANSION OF $\Sigma_1(\tau n^{-1})$

Since $\lambda_+(\omega,\tau n^{-1})$ is even in τn^{-1}, the function

$$\Sigma_1(\tau n^{-1}) = \int_0^1 d\omega(1-\omega^2)^{-1/2}\ln\lambda_+(\omega,\tau n^{-1}) - 2\int_0^1 d\omega(\tau^2n^{-2}+\omega^2)^{1/2}\ , \tag{C1}$$

is also even in τn^{-1}. Therefore, it has the asymptotic expansion

$$\Sigma_1(\tau n^{-1}) = \Sigma_1(0)+\tfrac{1}{2}\tau^2n^{-2}\Sigma_1''(0)+R(\tau n^{-1})\ , \tag{C2}$$

in which

$$\begin{aligned}\Sigma_1(0) &= \int_0^1 d\omega(1-\omega^2)^{-1/2}\ln\lambda_+(\omega,0)-2\int_0^1 d\omega\,\omega\\ &= \int_0^1 d\omega(1-\omega^2)^{-1/2}\ln[1+2\omega^2+2\omega(1+\omega^2)^{1/2}]-1\\ &= 2G-1\end{aligned} \tag{C3}$$

and

$$\begin{aligned}\Sigma_1''(0) &= \int_0^1 d\omega(1-\omega^2)^{-1/2}[\lambda_+''(\omega,0)/\lambda_+(\omega,0)]-2\int_0^1\omega^{-1}d\omega\\ &= 2\int_0^1 d\omega\,\omega^{-1}[(1-\omega^4)^{-1/2}-1]=\ln 2\ .\end{aligned} \tag{C4}$$

The remainder $R(\tau n^{-1})$ in the expansion (C2) can be put in the form

$$R(\tau n^{-1}) = \int_0^1 d\omega\,T(\omega,\tau n^{-1})\ , \tag{C5}$$

in which

$$T(\omega, \tau n^{-1}) = (1-\omega^2)^{-1/2}[\ln\lambda_+(\omega, \tau n^{-1}) - \ln\lambda_+(\omega, 0) - \tfrac{1}{2}\tau^2 n^{-2}\lambda_+''(\omega, 0)/\lambda_+(\omega, 0)] - [2(\tau^2 n^{-2}+\omega^2)^{1/2} - 2\omega - \tau^2 n^{-2}\omega^{-1}] \ . \tag{C6}$$

Consider first the contribution due to the integration over the interval $[0, c/n]$, namely,

$$R_1 = \int_0^{c/n} d\omega\, T(\omega, \tau n^{-1}) \ . \tag{C7}$$

In this interval, $X = (\tau^2 n^{-2} + \omega^2)^{1/2} \sim c/n$ is much less than unity and so we can expand $\ln\lambda_+(\omega, \tau n^{-1})$ as a Taylor series in $(\tau^2 n^{-2}+\omega^2)^{1/2}$. (Note that $\ln\lambda_+$ is analytic in X.) This yields

$$\ln\lambda_+(\omega, \tau n^{-1}) = 2(\tau^2 n^{-2}+\omega^2)^{1/2} + \tfrac{11}{3}(\tau^2 n^{-2}+\omega^2)^{3/2} + O(c^4 n^{-4}) \ , \tag{C8}$$

and, in particular,

$$\ln\lambda_+(\omega, 0) = 2\omega + \tfrac{11}{3}\omega^3 + O(c^4 n^{-4}) \ . \tag{C9}$$

On substituting (C8) and (C9) into (C6), we get

$$T(\omega, \tau n^{-1}) \approx (1-\omega^2)^{-1/2}\, \tfrac{11}{3}[(\tau^2 n^{-2}+\omega^2)^{3/2} - \omega^3] + 2[(1-\omega^2)^{1/2} - 1][(\tau^2 n^{-2}+\omega^2)^{1/2} - \omega] - \tfrac{1}{2}\tau^2 n^{-2}\{2\omega[(1-\omega^4)^{-1/2} - 1]\} \sim n^{-2}\tau^2\omega \ . \tag{C10}$$

Therefore R_1 defined in (C7) is of the order $n^{-4}c^2$, so that

$$R_1 \sim n^{-3} \quad \text{for} \quad c = n^{1/2} \ . \tag{C11}$$

Consider next the contribution due to the rest of the integration range, namely,

$$R_2 = \int_{c/n}^{1} d\omega\, T(\omega, \tau n^{-1}) \ . \tag{C12}$$

When $\omega \geq c/n$, we may expand $\lambda_+(\omega, \tau/n)$ as a Taylor series in τ/n to find

$$\lambda_+(\omega, \tau/n) - \lambda_+(\omega, 0) - \tfrac{1}{2}\tau^2 n^{-2}\lambda_+''(\omega, 0) = 2(\tau^2 n^{-2}+\omega^2)^{1/2}(1+\tau^2 n^{-2}+\omega^2)^{1/2} - 2\omega(1+\omega^2)^{1/2} - \tau^2 n^{-2}(1+\omega^2)^{-1/2}\omega^{-1}(1+2\omega^2) \sim n^{-1}c^{-3} \sim n^{-5/2} \ . \tag{C13}$$

We also find

$$2(\tau^2 n^{-2}+\omega^2)^{1/2} - 2\omega - \tau^2 n^{-2}\omega^{-1} \sim n^{-1}c^3 \sim n^{-5/2} \ . \tag{C14}$$

Consequently the balance of the remainder satisfies

$$R_2 \sim n^{-5/2} \ . \tag{C15}$$

This shows that the total remainder in (C5), which is a sum of R_1 and R_2, is of the order $n^{-5/2}$. Thus we have established the result

$$E_1(\tau n^{-1}) = 2G - 1 + \tfrac{1}{2}\tau^2 n^{-2}\ln 2 + O(n^{-5/2}) \ , \tag{C16}$$

quoted in (2.22).

APPENDIX D: THE CORRECTION TERM E_2

The correction term E_2, defined in (2.44), can be decomposed as

$$E_2 = (\pi n^2)^{-1}(E_2^A + E_2^B) \ , \tag{D1}$$

where

$$E_2^A = \int_0^c d\xi\, [(1-\xi^2 n^{-2})^{-1/2} - 1]\ln(p + q\, e^{-4X}) \ , \tag{D2}$$

and, with $\omega = \xi/n$,

$$E_2^B = \int_0^c d\xi\, (1-\xi^2 n^{-2})^{-1/2} \times \{\ln[v_+ + v_-\, e^{-n\xi} + z^2 u(1-e^{-n\xi})] - \ln(1+p^{-1}q\, e^{-4X})\} \ . \tag{D3}$$

Evidently one has the bound

$$|E_2^A| \leq [(1-c^2 n^{-2})^{-1/2} - 1]\int_0^c d\xi\, |\ln(p+q\, e^{-4X})| \ . \tag{D4}$$

Let us define

$$p_0(\xi) = 1 + \tau/X(\xi) \quad \text{and} \quad q_0(\xi) = 1 - \tau/X(\xi) \ . \tag{D5}$$

One sees that p_0 and q_0 are nonnegative for all τ and ξ. Since $(1-e^{-4X}) \leq 4X$ and $\sigma^2/X \geq 0$, we find

$$\ln(p+q\, e^{-4X}) = \ln[p_0 + q_0\, e^{-4X} + \sigma^2/X(1-e^{-4X})] \leq \ln(p_0 + q_0 + 4\sigma^2) = \ln(2+4\sigma^2) \ . \tag{D6}$$

Moreover, as q_0 is also nonnegative, we have

$$\ln(p+q\, e^{-4X}) \geq \ln p_0 \ . \tag{D7}$$

When $T > T_c (\tau > 0)$, we can see from (D.5) that p_0 exceeds unity, so that $\ln p_0 \geq 0$. Therefore $|\ln(p+q\, e^{-4X})| = \ln(p+q\, e^{-4X})$ for $T > T_c$. On substituting (D.6) into (D.4), we get

$$|E_2^A| \leq c^3 n^{-2}(1-c^2 n^{-2})^{-1/2}\ln(4+2\sigma^2) \ . \tag{D8}$$

On the other hand, when $T < T_c (\tau < 0)$, we have $p_0 \leq 1$, so that

$$-\ln p_0 \geq 0 \ . \tag{D9}$$

The bounds (D6), (D7), and (D9) yield

$$|\ln(p+q\, e^{-4X})| \leq \ln(4+2\sigma^2) - \ln p_0 \ . \tag{D10}$$

A straightforward integration then leads to

$$\int_0^c d\xi\, \ln p_0 \approx -c(c^{-1}\ln c) \quad \text{as} \quad c \to \infty \ . \tag{D11}$$

Hence, when $T < 0$, the error term E_2^A of (D4) satisfies

$$|E_2^A| \leq c^3 n^{-2}(1-c^2 n^{-2})^{-1/2}[\ln(2+4\sigma^2) + O(c^{-1}\ln c)] \sim n^{-1/2} \ . \tag{D12}$$

To discuss E_2^B we put

$$Q(\xi,\tau)=Q(\omega n,\tau)=v_+ + v_- e^{-n\xi}+z^2u(1-e^{-n\xi}),$$

$$Q_0(\xi)=Q(\xi,0), \tag{D13}$$

and

$$R(\xi,\tau)=p+q\,e^{-4X}, \quad R_0(\xi)=R(\xi,\tau) . \tag{D14}$$

Consequently, we can write E_2^B in the form

$$E_2^B=\int_0^c d\xi(1-\xi^2 n^{-2})^{-1/2}\cdot\{\ln v_+^0(\xi/n)+\ln[1+Y_1(\xi)] + \ln[1+Y_2(\xi,\tau)]\}, \tag{D15}$$

in which

$$v_\pm^0(\omega)=v_\pm(\omega,0)=1\pm\sqrt{2}\,\omega(1+\omega^2)^{-1/2}, \tag{D16}$$

$$Y_1(\xi)=Q_0(\xi)/v_+^0(\xi/n)R_0(\xi)-1, \tag{D17}$$

and

$$Y_2(\xi)=Q(\xi,\tau)R_0(\xi)/Q_0(\xi)R(\xi,\tau)-1 . \tag{D18}$$

We shall consider first the contribution to E_2^B arising from the integration of $\ln[1+Y_1(\xi)]$. By (D17) we have

$$Y_1(\xi)=R_0(\xi)^{-1}[(v_-^0/v_+^0-1)\,e^{-4\xi}+(v_-^0/v_+^0)\,e^{-4\xi}(e^{4\xi-n\xi^0}-1)+(z^2u^0/v_+^0-\sigma^2/\xi)(1-e^{-n\xi^0})+(\sigma^2/\xi)\,e^{-4\xi}(e^{4\xi-n\xi^0}-1)], \tag{D19}$$

where ξ^0 and u^0 denote $\xi(\omega,\tau)$ and $u(\omega,\tau)$ evaluated at $\tau=0$. It is easy to show that

$$|R_0(\xi)|\geq 1, \quad v_-^0/v_+^0\leq 1, \tag{D20}$$

$$|v_-^0/v_+^0-1|\leq 2\sqrt{2}\,\xi/n, \tag{D21}$$

and

$$z^2u^0/v_+^0-\sigma^2/\xi=\sigma^2/\xi\{(1-\omega^2)/[(1+\omega^2)^{1/2}+\sqrt{2}\,\omega]-1\}\approx(\sigma^2/\xi)\sqrt{2}\,\omega=\sqrt{2}(\sigma^2/n) . \tag{D22}$$

Furthermore, when $n^{-1}X$ is small, the function $e^{-n\xi(X)}$, given by (2.13) and (2.14), has a convergent Taylor expansion. Therefore, one finds

$$\begin{aligned} &e^{+4X-n\xi}-1\\ &=\exp\{4X-2n\ln[1+2n^{-2}X^2+2n^{-1}X(1+n^{-2}X^2)^{1/2}]\}-1\\ &=\tfrac{1}{3}n^{-2}X^3+O(n^{-3}X^4) . \end{aligned} \tag{D23}$$

This implies that there exists a positive constant M, such that

$$|e^{+4X-n\xi}-1|\leq n^{-2}X^3M . \tag{D24}$$

On substituting (D20)–(D22) and (D24) into (D19), we have

$$|Y_1(\xi)|\leq\sqrt{2}\,n^{-1}\xi\,e^{-4\xi}+n^{-2}\xi^3M\,e^{-4\xi} + 2(\sigma^2/n)+n^{-2}\xi^2M\sigma^2 . \tag{D25}$$

Because $\xi e^{-\xi}<1$, and $\xi^2\leq c^2=n$, we see that $|Y_1(\xi)|$ is of the order n^{-1}. Therefore

$$\left|\int_0^c \ln[1+Y_1(\xi)]\,d\xi\right|\approx c\,|Y_1(\xi)|\sim cn^{-1}=n^{-1/2} . \tag{D26}$$

We shall next show that $Y_2(\xi)$ of (D18) is also of the order n^{-1}. We write $Y_2(\xi)$ as

$$\begin{aligned} Y_2(\xi)=&\,Q_0(\xi)^{-1}R(\xi)^{-1}[(z^2u-\sigma^2/X)(1-e^{-n\xi})+(\sigma^2/X)e^{-4X}(1-e^{+4X-n\xi})]R_0(\xi)\\ &+Q_0(\xi)^{-1}R(\xi)^{-1}\{[v_+ + v_- e^{-n\xi}-(p+q\,e^{-4X})]R_0(\xi)-[v_+^0+v_-^0e^{-n\xi^0}-(1+e^{-4\xi})]R(\xi,\tau)\}\\ &-Q_0(\xi)^{-1}[(z^2u^0-\sigma^2/\xi)(1-e^{-n\xi^0})+(\sigma^2/\xi)\,e^{-4\xi}(1-e^{4\xi-n\xi^0})] . \end{aligned} \tag{D27}$$

As p_0, q_0, σ^2/X, and $(1-e^{-4X})$ are all nonnegative, we find

$$R(\xi)=p+q\,e^{-4X}\geq\sigma^2(1-e^{-4X})/X, \tag{D28}$$

$$R(\xi)\geq p_0+q_0\,e^{-4X}\geq e^{-4X}, \tag{D29}$$

and

$$R(\xi)\geq p_0\geq\tfrac{1}{2}\xi^2/X^2 . \tag{D30}$$

Using (2.6), we can show

$$|z^2u\,X/\sigma^2-1|\leq c^2n^{-2}[1+|\tau n^{-1}|+(\tau^2n^{-2}+2)^{1/2}]+2|\tau n^{-1}|+2\tau^2n^{-2}\sim n^{-1} . \tag{D31}$$

Moreover, from (D23) we find

$$(1-e^{-n\xi})\leq(1-e^{-4X}) . \tag{D32}$$

and by (D28), (D31), and (D32), we have

$$|R^{-1}(\xi)(z^2u-\sigma^2/X)(1-e^{-n\xi})|\sim n^{-1}\,. \tag{D33}$$

Using (D24) and (D29), we find

$$|R^{-1}(\xi,\tau)\,e^{-4X}\sigma^2(1-e^{4X-n\xi})/X|\leqslant\sigma^2Mn^{-2}X^2\leqslant M\sigma^2n^{-2}(\tau^2+c^2)\sim n^{-1}\,. \tag{D34}$$

Furthermore, it is trivial to establish

$$Q_0^{-1}(\xi)\leqslant 1 \quad\text{and}\quad |R_0(\xi)|<4+2\sigma^2\,. \tag{D35}$$

Combining (D33)–(D35), we find that the first term of $Y_2(\xi,\tau)$ in (D27) is of order n^{-1}.

Similarly, we can show that the last term of $Y_2(\xi,\tau)$, in (D27), is also of the order n^{-1}.

Since $(v_+-p_0)=-(v_--q_0)$, and $Q_0^{-1}(\xi)\leqslant 1$, the second term in (D27) becomes

$$\begin{aligned}
&Q_0(\xi)^{-1}R(\xi,\tau)^{-1}\{R_0(\xi)[(v_+-p_0)(1-e^{-n\xi})+q_0(e^{-n\xi}-e^{-4X})]-R(\tau,\xi)[(v_+^0-1)(1-e^{-n\xi^0})+(e^{-n\xi^0}-e^{-4\xi})]\}\\
&\quad\leqslant|v_+-p_0-v_+^0+1|+R^{-1}(\xi,\tau)|v_+-p_0|[|(1+e^{-4\xi})(1-e^{-n\xi})-(1-e^{-n\xi^0})(1+e^{-4X})|\\
&\qquad+(1-e^{-n\xi})\sigma^2(1-e^{-4\xi})/\xi+X^{-1}(\sigma^2+|\tau|)(1-e^{-n\xi^0})(1-e^{-4X})]+(e^{4\xi-n\xi^0}-1)R^{-1}(\xi,\tau)\\
&\qquad\times[|e^{-4X}-e^{-4\xi}|+e^{-4\xi}|\tau+\sigma^2|(1-e^{-4X})/X]+e^{-4X}R(\xi,\tau)^{-1}[|\tau|X^{-1}(e^{4X-n\xi}-1)|R_0(\xi)|\\
&\qquad+(1+e^{-4X})|e^{4X-n\xi}-e^{4\xi-n\xi^0}|+\sigma^2(e^{4X-n\xi}-1)(1-e^{-4\xi})/\xi]\,.
\end{aligned} \tag{D36}$$

From (2.5) and (D5), we can show

$$|v_+-p_0+v_+^0-1|\leqslant 2n^{-2}\xi\tau+2|\tau|n^{-1}+O(n^{-3})\sim n^{-1} \tag{D37}$$

and

$$|v_+-p_0|\leqslant 2n^{-1}\xi^2X^{-1}\,. \tag{D38}$$

Using (D30) and (D38), we find,

$$|R^{-1}(\xi,\tau)(v_+-p_0)|\leqslant 4n^{-1}X\,. \tag{D39}$$

Because $\xi e^{-\xi}<1$, and $X\leqslant|\tau|+\xi$, we have

$$|(1-e^{-n\xi})(1+e^{-4\xi})-(1-e^{-n\xi^0})(1+e^{-4X})|\leqslant 4e^{-4\xi^0}\leqslant X^{-1}. \tag{D40}$$

Furthermore, we can write

$$\begin{aligned}(1-e^{-4\xi})\xi^{-1}&=(1-e^{-4\xi})(X^{-1}+\xi^{-1}-X^{-1})\\
&\leqslant X^{-1}+\xi^{-1}X^{-2}\tau^2(1-e^{-4\xi})\leqslant X^{-1}(1+4\tau)\,.\end{aligned} \tag{D41}$$

By (D25) and (D30), we get

$$\xi^{-1}R^{-1}(\xi,\tau)(e^{4\xi-n\xi^0}-1)\leqslant 2Mn^{-2}X^2\sim n^{-1}\,. \tag{D42}$$

We also have the bound

$$\xi|e^{-4X}-e^{-4\xi}|\leqslant 2\xi\,e^{-4\xi}<1\,. \tag{D43}$$

Finally, by (D23), we have $R(\xi,\tau)^{-1}e^{-4X}\leqslant 1$ and also find

$$e^{4X-n\xi}-e^{4\xi-n\xi^0}\approx\tfrac{1}{3}n^{-2}(X^3-\xi^3)\leqslant\tfrac{2}{3}n^{-2}X^2\tau\sim n^{-1}\,. \tag{D44}$$

The bound (D24), leads to

$$X^{-1}(e^{4X-n\xi}-1)\leqslant Mn^{-2}X^2\sim n^{-1}\,, \tag{D45}$$

and, with (D41), to

$$(e^{4X-n\xi}-1)(1-e^{-4\xi})/\xi\sim n^{-1}\,. \tag{D46}$$

This shows that every term in (D36) is of the order n^{-1}. Therefore we have $Y_2(\omega,\tau)\sim n^{-1}$, and hence obtain

$$\left|\int_0^c d\xi\,(1-\xi^2n^{-2})\ln[1+Y_2(\omega,\tau)]\right|\sim cn^{-1}\sim n^{-1/2}\,. \tag{D47}$$

Consequently, we have established the estimate

$$E_2=(\pi n)^{-1}\int_0^{c/n}d\omega\,(1-\omega^2)^{1/2}\ln v_+(\omega,0)+O(n^{-5/2})\,, \tag{D48}$$

and, since by the definition (2.33), we also have

$$E_3=-(\pi n)^{-1}\int_0^{c/n}d\omega\,(1-\omega^2)^{1/2}\ln v_+(\omega,0)\,, \tag{D49}$$

we conclude that (E_2+E_3) is of the order $n^{-5/2}$.

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