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Finite-Size Effects in Surface Tension. I. Fluctuating Interfaces

D. B. Abraham[1,2] and N. M. Švrakić[1]

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We consider a two-dimensional Ising cylinder of circumference M and height N, with a floating interface introduced by the appropriate boundary conditions. An exact analysis of the finite-size effects in surface tension is given and the scaling function for all temperatures is calculated. The results are compared with the Monte Carlo data of Mon and Jasnow.

KEY WORDS: Ising model; interfaces; finite-size effects; Monte Carlo.

1. INTRODUCTION

The statistical mechanical behavior of a domain wall (interface) between coexisting phases in a confined geometry is a subject of considerable theoretical importance in constructing definitions of surface tension which are amenable to exact investigation. In this paper, we are concerned with one such definition, due originally to Fisher,[1] which has been partially investigated elsewhere.[2] Our interest in this area was rekindled by the Monte Carlo investigation of Mon and Jasnow[3] of surface tension and in particular the amplitude ratios (believed to be correct for arbitrary dimension d),

$$\tau_0 \xi_0^{d-1} = c(d) \tag{1.1}$$

where the nonuniversal amplitude τ_0 is associated with the critical behavior of the surface tension $\tau \sim \tau_0 t^{\mu}$, with $t \equiv (T_c - T)/T_c$. Similarly, the correlation length behaves as $\xi \sim \xi_0 t^{-\nu}$. The number $c(d)$ is lattice-independent.

[1] HLRZ-KFA, Postfach 1913, D-5170, Jülich, Germany.
[2] On leave from: Department of Theoretical Chemistry, Oxford University, Oxford, OX1 3UB, England.

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The critical exponents are related by Widom's scaling relation $(d-1)\,\nu=\mu$. This was derived[4] by a *local* fluctuation analysis using equipartition and dating from before the demise of the van der Waals theory of the interface structure; exact calculation for the planar Ising model established rigorously[5] that the interface fluctuates for all subcritical temperatures, making Widom's analysis incomplete. Thus, a nonlocal definition of surface tension appeared desirable, and several were given and proved to make sense.[5] One such, based on symmetry-breaking or Dobrushin boundary conditions,[6] gives (1.1) directly from duality for $d=2$, with $c(2)=1/2$; we shall return to this point later, after mentioning the finite-size scaling ansatz for the surface tension; this is[5]

$$\tau=\tau_0 t^{\mu}\Sigma(Lt^{\nu}c) \tag{1.2}$$

for a lattice of size L, where the function $\Sigma(x)$ satisfies $\Sigma(\infty)=1$, $\Sigma(x)\sim x^{-\mu/\nu}$ for small x; the number c depends on the lattice type, but $\Sigma(x)$ is thought to be a universal function for each dimension. Such scaling forms are of crucial importance if one wants to extract thermodynamic limiting information from necessarily finite-size Monte Carlo data. For the $2D$ system, Mon and Jasnow[5] used the form (which we will show to be an approximate one)

$$\Sigma(x)=1+\frac{B}{x} \tag{1.3}$$

with $\mu=\nu=1$, to fit their Monte Carlo data. We will derive the exact form of $\Sigma(x)$ in (1.3) for the geometry used by Mon and Jasnow; we also consider other finite-size properties of fluctuating interfaces. Some of the results presented here have been previously published in shorter form.[7]

To specify the problem, consider a ferromagnetic Ising model on a $2D$ square lattice wrapped on the cylinder of length N and circumference M. The nearest-neighbor couplings parallel to the cylinder axis are K_1, while those in the other direction are K_2. (Throughout this work we will always assume $T<T_c$, unless otherwise stated, as in Section 5.) The $+-$ boundary conditions at the faces of the cylinder in the thermodynamic limit $N\to\infty$, $M\to\infty$, with M and N appropriately related, for low enough temperatures, induce exactly one domain wall with probability one. Similarly, the $++$ boundary conditions induce no domain walls in the same limit. It is crucial here that N should not grow too fast with M.

Thus, a potential definition of the surface tension (per spin, scaled by $k_{\mathrm{B}}T$) is

$$\tau=\lim_{M,N\to\infty}\tau(M,N), \qquad M, N \text{ related} \tag{1.4}$$

where

$$\tau(M, N) = -\frac{1}{M} \ln\left(\frac{Z^{(+-)}}{Z^{(++)}}\right) \tag{1.5}$$

with Z being the partition function, and the superscript specifying the boundary conditions. The amplitude relation (1.1) for this definition is not an obvious consequence of duality. Indeed, the dual of Z^{+-}/Z^{++} in (1.5) is a Wilson loop on a cylinder with free boundary conditions on its ends. This suggests (1.1), but does not help in the evaluation of the scaling form. In what follows we calculate exactly $\tau(M, N)$ and analyze its finite-size behavior. In Section 2, we develop necessary mathematical preliminaries needed to express (1.5) in a form such that its finite-size behavior can be analyzed. This analysis is given in Section 3. Section 4 presents discussion of the behavior of the interface in the scaling limit. Here we give the complete form of the scaling function. Section 5 discusses the behavior of the interface for temperatures above T_c. Finally, in the Appendix A we describe the evaluation of a useful infinite product, while Appendices B and C contain various mathematical details used in the analysis.

2. DEVELOPMENT OF MODEL

We start from the definition (1.5) for the finite-size surface tension. The appropriate partition functions in (1.5) can be evaluated by the use of the transfer matrix method. Specifically, (1.5) can be expressed in the form

$$\tau(M, N) = \frac{1}{M} \ln\left(\frac{\langle - | V^N | + \rangle}{\langle + | V^N | + \rangle}\right) \tag{2.1}$$

where we use the usual symmetrized transfer matrix

$$V = V_2^{1/2} V_1 V_2^{1/2} \tag{2.2}$$

with

$$V_2 = \exp\left(K_2 \sum_{j=1}^{M} \sigma_j^x \sigma_{j+1}^x\right) \tag{2.3}$$

and

$$V_1 = \exp\left(-K_1^* \sum_{j=1}^{M} \sigma_j^z\right) \tag{2.4}$$

In the above, σ^α ($\alpha = x, y, z$) are Pauli matrices, while K_i^* ($i = 1, 2$) is the dual coupling defined by $\sinh 2K_i \sinh 2K_i^* = 1$. (Note that, even though we use the quantum mechanical notation, our model is fully classical.) The boundary states are given by

$$\sigma_j^x |\pm\rangle = +|\pm\rangle \tag{2.5}$$

for all j with $1 \leqslant j \leqslant M$. These states are constructed from the maximal eigenvalues of V_2, written in terms of the spinors used in the usual methods of diagonalizing V. Note that V_2 commutes with the operator

$$P_M = \prod_{j=1}^{M} (-\sigma_j^z) \tag{2.6}$$

which is a rotation by π about the z axis, up to a factor. This has the important consequence that

$$P_M |+\rangle = |-\rangle \tag{2.7}$$

if we define

$$|\pm\rangle = 2^{-M/2} \prod_{j=1}^{M} (1 \pm \sigma_j^x)\, |0\rangle \tag{2.8}$$

where $\sigma_j^z |0\rangle = -|0\rangle$ for all j with $1 \leqslant j \leqslant M$. We now introduce the Fermi operators

$$f_j = P_{j-1} \sigma_j^-, \qquad j = 1, 2,..., M \tag{2.9}$$

with

$$P_j = \prod_{k=1}^{j} (-\sigma_k^z), \qquad P_0 = 1 \tag{2.10}$$

The transfer operator now takes the form

$$V_2 = \exp K_2 \left\{ \sum_{j=1}^{M-1} (f_j^\dagger - f_j)(f_{j+1}^\dagger + f_{j+1}) - P_M(f_M^\dagger - f_M)(f_1^\dagger + f_1) \right\} \tag{2.11}$$

When projected onto the invariant subspace of P_M, which actually selects the parity of the fermion number, V_2 becomes the exponential of the quadratic form

$$V_2 = \tfrac{1}{2}(1 + P_M)\, V_2(+) + \tfrac{1}{2}(1 - P_M)\, V_2(-) \tag{2.12}$$

We introduce the transformed fermions by

$$F_{\omega}^{\dagger}=M^{-1/2}\sum_{j=1}^{M}e^{i\omega j}f_{j}^{\dagger} \tag{2.13}$$

where $e^{i\omega M}=\pm 1$; the antiperiodic wavenumbers appear when P_M is replaced by 1 as in $V_2(+)$. Provided we deal exclusively with periodic or antiperiodic wavenumbers, it is easy to check that (2.13) is canonical. A simple exercise shows that

$$|\Phi_{+}^{0}\rangle=\prod_{>0}^{<\pi}[\cos\theta_0(\omega)+i\sin\theta_0(\omega)\,F_{-\omega}^{\dagger}F_{\omega}^{\dagger}]\,|0\rangle \tag{2.14}$$

with $\exp(i\omega M)=-1$, and

$$|\Phi_{-}^{0}\rangle=F_{0}^{\dagger}\prod_{>0}^{<\pi}[\cos\theta_0(\omega)+i\sin\theta_0(\omega)\,F_{-\omega}^{\dagger}F_{\omega}^{\dagger}]\,|0\rangle \tag{2.15}$$

with $\exp(i\omega M)=1$ and $\theta_0(\omega)=(\pi+\omega)/2$, mod π, are indeed maximal eigenvectors of $V_2(\pm)$, respectively. Including the projectors in (2.12), they are also eigenvectors of V_2 itself. Clearly, we have

$$|\Phi_{+}^{0}\rangle=a|+\rangle+b|-\rangle \tag{2.16}$$

$$|\Phi_{-}^{0}\rangle=c|+\rangle+d|-\rangle \tag{2.17}$$

Since the vectors are in different invariant subspaces of P_M, we have $\langle\Phi_{+}^{0}|\Phi_{-}^{0}\rangle=0$. Thus,

$$ac+bd=0 \tag{2.18}$$

Since $P_M|\Phi_{\pm}^{0}\rangle=\pm|\Phi_{\pm}^{0}\rangle$, from (2.7) we have

$$a=b \qquad \text{and} \qquad c=-d \tag{2.19}$$

which guarantees (2.18). Normalization gives

$$|\Phi_{\pm}^{0}\rangle=2^{-1/2}e^{i\varphi_{\pm}}(|+\rangle\pm|-\rangle) \tag{2.20}$$

where $\varphi_{\pm}$ are as yet undetermined phase factors. By equating coefficients of $|0\rangle$ in (2.20) for $|\Phi_{+}^{0}\rangle$ we have

$$e^{i\varphi_{+}}=2^{(M-1)/2}(-1)^{M}\prod_{>0}^{<\pi}\sin(\omega/2); \qquad e^{i\omega M}=-1 \tag{2.21}$$

from which it follows that

$$e^{i\varphi_{+}}=(-1)^{M} \tag{2.22}$$

In the case of $|\Phi_{-}^{0}\rangle$ we equate coefficients of $F_0^\dagger|0\rangle$ in (2.21), giving

$$e^{i\varphi_-}=(-1)^M \tag{2.23}$$

Thus, (2.1) is reduced to

$$\tau(M,N)=\frac{1}{M}\ln\left\{\frac{P_N(+)-P_N(-)}{P_N(+)+P_N(-)}\right\} \tag{2.24}$$

where

$$P_N(\pm)=\langle\Phi_{\pm}^{0}|\,V^N(\pm)\,|\Phi_{\pm}^{0}\rangle \tag{2.25}$$

are now in a form suitable for evaluation by the spinor method. A straightforward calculation (see Appendix) gives

$$P_N(+)=\prod_{>0}^{<\pi} f_N(\omega) \tag{2.26}$$

with $\exp(iN\omega)=-1$, whereas

$$P_N(-)=\exp\left\{\frac{1}{2}N[\gamma(0)+\gamma(\pi)]\right\}\prod_{>0}^{<\pi} f_N(\omega) \tag{2.27}$$

with $\exp(iN\omega)=+1$, and we have assumed M to be even; the generalization to odd M is essentially trivial. In the above, $\gamma(\omega)$ is Onsager's function[8] given by

$$\cosh\gamma(\omega)=\cosh 2K_1^*\cosh 2K_2-\sinh 2K_1^*\sinh 2K_2\cos\omega \tag{2.28}$$

with $\gamma(\omega)\geqslant 0$ for real ω. The function $f_N(\omega)$ is given by

$$f_N(\omega)=\cosh N\gamma(\omega)+\sinh N\gamma(\omega)\cos\delta^*(\omega) \tag{2.29}$$

where $\delta^*(\omega)$ is an angle of Onsager's hyperbolic triangle[8] given by

$$\begin{aligned}\sinh\gamma(\omega)&\cos\delta^*(\omega)\\&=\sinh 2K_2\cosh 2K_1^*-\sinh 2K_1^*\cosh 2K_2\cos\omega\end{aligned} \tag{2.30}$$

and

$$\sinh\gamma(\omega)\sin\delta^*(\omega)=\sinh 2K_1^*\sin\omega \tag{2.31}$$

Using these results, (2.24) is reduced to

$$\tau(M,N)=\frac{1}{M}\ln\left\{\frac{T(M,N)-1}{T(M,N)+1}\right\} \tag{2.32}$$

where

$$T(M, N) = \exp\left\{\frac{1}{2}\left(\sum_{+} - \sum_{-}\right) \ln f_N(\omega)\right\} \tag{2.33}$$

where $\sum_{+}$ and $\sum_{-}$ are sums over ω in $(-\pi, \pi]$ such that $\exp(iM\omega) = -1$ or $+1$, respectively.

From simple complex variable theory

$$\sum_{\pm} \ln f_N(\omega) = \mp \frac{M}{2\pi} \oint_C \frac{d\omega}{e^{iM\omega} \pm 1} \ln f_N(\omega) \tag{2.34}$$

where C winds once around zeros of $e^{iM\omega} \pm 1$, but not around any singularities of $\ln f_N(\omega)$. The last step is feasible, as we shall show in the next section. Inserting (2.34) into (2.33) gives

$$T(M, N) = \exp\left\{-\frac{M}{4\pi i} \oint_C \frac{d\omega}{\sin M\omega} \ln f_N(\omega)\right\} \tag{2.35}$$

which is the key equation for analyzing finite-size effects. Before going on to that, however, let us return briefly to (2.1) and (2.24) and (2.25). It is often stated that the surface tension is given just by studying the ratio of the two largest eigenvalues. There is, however, no reason in the spectral decomposition of $V(\pm)^N$ in (2.24) and (2.25) why the difference between higher-order terms in the dispersion should not dominate the lowest ones in the asymptotics. Further, the matrix element $\langle \Phi^0_\pm \mid \Phi_\pm \rangle$ would have to be investigated carefully and this would demand a thorough analysis of the thermodynamic-limiting procedure. Fortunately, Eq. (2.26) contains an *implicit* summation of the dispersion series and it is to the analysis of this product that we return in the next section.

3. ANALYSIS

Using the even character of $f_N(\omega)$, (2.35) becomes

$$T(M, N) = \exp\left\{\frac{M}{2\pi i} \int_{-\pi + i\varepsilon}^{\pi + i\varepsilon} \frac{d\omega}{\sin M\omega} \ln f_N(\omega)\right\} \tag{3.1}$$

for $\varepsilon > 0$ small enough. Using (2.29), $\ln f_N(\omega)$ has logarithmic branch points whenever

$$\cosh N\gamma(\omega) + \sinh N\gamma(\omega) \cos \delta^*(\omega) = 0 \quad (\text{or } \infty) \tag{3.2}$$

With (2.30)–(2.31), (3.2) becomes

$$e^{2N\gamma(\omega)} = \frac{1}{AB} \frac{(e^\gamma - A)(e^\gamma - B)}{(e^\gamma - A^{-1})(e^\gamma - B^{-1})} \tag{3.3}$$

where

$$A = \exp[2(K_2 + K_1^*)], \qquad B = \exp[2(K_2 - K_1^*)] \tag{3.4}$$

We expect $2(N+1)$ solutions to this equation in the variable $e^{-\gamma}$. First, note that if $z = e^\gamma$ is a solution, then z^{-1} is also a solution, and that $e^{-\gamma} = \pm 1$ are solutions. We seek solutions for $0 \leqslant T < T_c$: For $\gamma = it$, $t \in \mathfrak{R}$, (3.3) becomes

$$\exp(2Nit) = \exp[2i\hat{\delta}'(t)] \tag{3.5}$$

where $\hat{\delta}'(\omega)$ is another hyperbolic-triangular angle introduced by Onsager[8]:

$$\sinh\gamma(\omega)\cos\hat{\delta}'(\omega) = \sinh 2K_2^* \cosh 2K_1 - \cosh 2K_2^* \sinh 2K_1 \cos\omega \tag{3.6}$$

and

$$\sinh\gamma(\omega)\sin\hat{\delta}'(\omega) = \sinh 2K_2 \sin\omega \tag{3.7}$$

We take the branch of (3.6) and (3.7) with $|\hat{\delta}'(t)| \leqslant \pi$. It is easy to see that $\hat{\delta}'(\pi) = 0$, $\hat{\delta}'(\omega)$ is 2π-periodic, and that $\hat{\delta}'(0\pm) = \pm\pi$. Equation (3.5) is of the form

$$Nt - j\pi = \hat{\delta}'(t) \tag{3.8a}$$

where j is any integer. Looking for a solution in $(0, \pi)$, it is clear from an elementary fixed-point argument that there is a unique solution for each integer j on $[0, N]$ with $\pi j/N < t_j < \pi(j+1)/N$. For $j = \pm 1$ it is clear that $t = 0$ is also a solution. On $[-\pi, 0)$, for integer j on $[-N, 0]$, there is a unique solution with $\pi(j-1)/N < t_j < \pi j/N$, but that $t_j = -t_{-j}$. Note the special case $t_{\pm N} = \pi \pmod{2\pi}$. Thus, we get $2N$ complex unimodular solutions of (3.3) for e^γ, and the solution $e^\gamma = \pm 1$, completing the set. As far as (3.1) is concerned, $e^\gamma = \pm 1$ do not generate logarithmic branch points and are thus trivial. Provided $|\cos\hat{\delta}'| > 0$, one can check that the Newton–Raphson procedure for root location converges rapidly: (3.5) gives

$$t_j = \frac{j\pi}{N} + \frac{1}{N}\hat{\delta}'\left(\frac{j\pi}{N}\right) + O\left(\frac{1}{N^2}\right) \tag{3.8b}$$

for $j=0, 1,..., 2N-1$. Equations (3.5) and (2.28) give

$$\cos \omega_j = \frac{\cosh 2K_1^* \cosh 2K_2 - \cos t_j}{\sinh 2K_1^* \sinh 2K_2} \tag{3.9}$$

Clearly ω_j is pure imaginary (in the strip $|\Re\omega| \leqslant \pi$): if $\omega = iv_j$, then

$$\cosh v_j = \cosh 2K_1 \cosh 2K_2^* - \sinh 2K_1 \sinh 2K_2^* \cos\left(\frac{j\pi}{N}\right) + O\left(\frac{1}{N}\right) \tag{3.10}$$

Thus (3.1) gives

$$T(M, N) = \exp\left\{M \sum_{j=1}^{N-1} \int_{v_j(N)}^{\infty} \frac{dv}{\sinh Mv}\right\} \tag{3.11}$$

by analyzing the behavior of $f_N(\omega)$ round its branch cuts. The integral is basic, giving

$$T(M, N) = \exp\left\{-\sum_{j=1}^{N-1} \ln\left(\tanh \frac{1}{2} Mv_j\right)\right\} \tag{3.12}$$

We shall examine some special cases of this formula:

Result 1. $M \to \infty$, N fixed: Since for $j=1, 2,..., N-1$, we have $v_{j+1} > v_j$, only v_1 appears, i.e.,

$$\lim_{M\to\infty} \frac{1}{M} \ln\left(\frac{T(M, N)-1}{T(M, N)+1}\right) = -v_1(N) \tag{3.13}$$

Referring to (3.10), we have

$$\cosh v_1(N) = \cosh 2(K_1 - K_2^*) + \sinh 2K_1 \sinh 2K_2^* \frac{\pi^2}{2N^2} + O\left(\frac{1}{N^4}\right) \tag{3.14a}$$

from which, *provided* $4N(K_1 - K_2^*) \gg 1$, that is, *the system is much wider than the correlation length,*

$$v_1(N) = 2(K_1 - K_2^*) + u\frac{\pi^2}{2N^2} + O\left(\frac{1}{N^4}\right) \tag{3.14b}$$

The first term on the right is the Onsager surface tension.[8] In the second, we have

$$u = \frac{\sinh 2K_1 \sinh 2K_2^*}{\sinh 2(K_1 - K_2^*)} \tag{3.15}$$

so that $1/u \equiv \kappa$ is the *surface stiffness coefficient*. This $1/N^2$ term is the "entropic repulsion" advocated by Fisher and Fisher[9] using random-walk arguments. We provide a rigorous derivation here for the planar Ising model. What this does is to specify random-walk parameter values determined from molecular-level considerations. An equivalent approach is via a solid-on-solid, or capillary wave, model[5] which may be thought of as a *gedanken* renormalization of the interface between two extremal Ising ferromagnetic phases, replacing bare spin–spin coupling by the stiffness coefficient u. Our qualification on (3.14b) provides a physically-anticipated limit to validity of the random-walk type of theory. Note also that (3.14) agrees precisely with the capillary-wave prediction.

It has been known for some time[17] that the interface of length M has fluctuations of the order of $\sqrt{M}$ in extent about its mean location. Thus, we anticipate crossover behavior if the limit $M \to \infty$, $N \to \infty$ is taken so that $N/M^{1/2} = \alpha$ is fixed.

Result 2. For $\alpha > 0$ and $K_1 > K_2^*$ we have

$$\lim_{M \to \infty} M[\tau(M, \alpha M^{1/2}) - 2(K_1 - K_2^*)]$$

$$= -\ln \sum_{j=1}^{\infty} \exp[-(\pi j)^2 u/2\alpha^2] \equiv F(\alpha) \tag{3.16}$$

Intuitively speaking, this result follows easily from the large-M asymptotics of (3.12),

$$|T(M, N) - P| \leqslant PM^{1/2} e^{-3Mv_0} \tag{3.17a}$$

$$P = \exp\left(2 \sum_{1}^{N-1} e^{-Mv_j}\right) \tag{3.17b}$$

Equation (3.10) gives

$$\cosh v_j(N) = \cosh 2(K_1 - K_2^*) + \sinh 2K_1 \sinh 2K_2^* \left(1 - \cos \frac{j\pi}{N}\right) \tag{3.18}$$

so for $j \ll N$, we have, roughly speaking

$$v_j(N) = 2(K_1 - K_2^*) + u \frac{\pi^2 j^2}{2N^2} \tag{3.19}$$

valid provided $j \ll N[2(K_1 - K_2^*)/u]^{1/2}$, and so

$$\frac{T(M, N) - 1}{T(M, N) + 1} \sim [\exp(-Mv_0)] \sum_{j=1}^{\infty} \exp\left[-u\left(\frac{\pi^2 j^2}{2\alpha^2}\right)\right] \tag{3.20}$$

from which Result 2 follows directly. In Appendix B we give a complete derivation of (3.16).

For α small, the first term in the sum (3.16) dominates, giving $F(\alpha) = \pi^2 u/2\alpha^2$; this recaptures (3.14). For α large, the Poisson summation formula gives $F(\alpha) = \ln \alpha + O(1)$.

Result 3. If the height N of the cylinder grows faster, say as αM^δ with $\delta > 1/2$, then we get

$$\tau(M, \alpha M^\delta) = v_0 + \frac{\ln M}{M} + O\left(\frac{1}{M}\right) \tag{3.21}$$

Result 4. If $N = \alpha M^\delta$, $\delta < 1/2$, then we get

$$\tau(M, \alpha M^\delta) \sim v_0 + \frac{u\pi^2}{M^{2\delta}} + O\left(\frac{1}{M^{2\delta}}\right) \tag{3.22}$$

which is consistent with the entropic repulsion idea.

The reader will no doubt have noticed that the physical thinking behind the first few results is that *there is a single domain wall induced by the + − boundary conditions on the cylinder*. This could be investigated by determining the magnetization along the cylinder in finite geometry: the number of changes of sign of the magnetization is the number of domain walls. Such a study is feasible in principle, but the details of the calculation are beyond the scope of this article.

If the cylinder height N grows sufficiently fast with M, or indeed if M is finite but $N \to \infty$, we expect domain walls to proliferate. [The potential proliferation of domain walls was anticipated by Fisher *et al.*[10] and placed on a more precise footing by Privman and Fisher[11] and Brezin and Zinn-Justin.[12] The result (3.25) below is rigorous.] Thus, it is possible that $T(M, N)$ diverges, giving a vanishing surface tension. Equation (3.17) contains a key to this: as $N \to \infty$, the sum in (3.17) can be approximated by a Riemann integral. First, (3.18) and (2.28) give $v_j(N) \sim \hat{\gamma}(\pi j/N)$, where $\hat{\gamma}$ is as γ in (2.28), but with K_1 and K_2 interchanged. Thus,

$$T(M, N) \sim \exp\left\{\frac{N}{2\pi}\int_{-\pi}^{\pi} e^{-M\hat{\gamma}(\omega)}\, d\omega\right\} \tag{3.23}$$

Suppose now $N = e^{\lambda M}$, with $\lambda > 0$: as $M \to \infty$, we have

$$\ln T(M, N) \sim e^{M(\lambda - \hat{\gamma}(0))}\left(\frac{2\pi}{M\hat{\gamma}^{(2)}(0)}\right)^{1/2}\left\{1 + O\left(\frac{1}{M}\right)\right\} \tag{3.24}$$

Result 5. We have

$$\lim_{M\to\infty} \tau(M, e^{\lambda M}) = \begin{cases} 0 & \text{for} \quad \lambda > \hat{\gamma}(0) \\ \hat{\gamma}(0) - \lambda & \text{for} \quad 0 \leqslant \lambda < \hat{\gamma}(0) \end{cases} \tag{3.25}$$

Although the full treatment of the domain-wall content in this system is beyond the scope of the present article, we can give two elementary explanations of (3.25).

Intuitively, the asymptotic decay of the pair correlation function $\langle \sigma(1, 1)\, \sigma(1, y) \rangle$ along the axis of the cylinder is governed by Λ_1/Λ_0, where $\Lambda_0 > \Lambda_1 > \cdots$ are the eigenvalues of the transfer matrix along the cylinder axis. The correlation length is[11]

$$\xi_{\parallel} = \frac{1}{\ln(\Lambda_0/\Lambda_1)} \tag{3.26}$$

which gives

$$\xi_{\parallel} \sim \sqrt{M}\, e^{M\tau} \tag{3.27}$$

Thus, if $N \ll e^{M\tau}$, we get a single domain wall, whereas if $N \sim e^{\lambda M}$ with $\lambda > \tau$, the number of domain walls should diverge with M.

Another argument is to say that the domain walls do not cross, so that they can be regarded as fermions in one dimension. The partition function for n of these in a length N is roughly $Z_0^n(M)\binom{N}{n}$, where $Z_0(M)$ is the partition function for a single loop on a cylinder of circumference M when free translation has been suppressed. Studying the n which maximizes this partition function leads back to the same picture.

4. SCALING RESULTS

Let us scale the cylinder dimensions by the appropriate correlation lengths for the bulk phases with $T < T_c$. Wu[13] showed that the correlation lengths along the axis ($\xi_{\parallel}$) and perpendicular to it ($\xi_{\perp}$) are given in the bulk by

$$\xi_{\parallel} = \frac{1}{4(K_2 - K_1^*)}, \qquad \xi_{\perp} = \frac{1}{4(K_1 - K_2^*)} \tag{4.1}$$

We take the scaling limit N, $M \to \infty$ with $T \to T_c^-$ (i.e., $K_1^* \to K_2^-$) such that $\tilde{N} = N/\xi_{\parallel}$ and $\tilde{M} = M/\xi_{\perp}$ are fixed. We define this limit as s-lim.

Let us examine the scaling behavior of (3.12) and (3.2). It is easy to see that if

$$u = \sinh 2K_c \left\{ s\text{-lim} \left(\frac{\omega}{\gamma(0)} \right) \right\} = 2\{ s\text{-lim}(\omega \xi_{\perp}) \} \tag{4.2}$$

where s-lim is extended to the coupled limit also with $\omega \to \infty$, then (3.2) becomes

$$\cosh\left[\frac{\tilde{N}}{2}(1+u^2)^{1/2}\right]+\frac{1}{(1+u^2)^{1/2}}\sinh\left[\frac{\tilde{N}}{2}(1+u^2)^{1/2}\right]=0 \tag{4.3}$$

This only has solutions nontrivial in the sense of the branch cut analysis, if $(1+u^2)^{1/2}$ is pure imaginary. Denote

$$(1+u^2)^{1/2} = \pm iz_j \tag{4.4}$$

Then (4.3) becomes

$$\tan\frac{\tilde{N}z}{2} = -z \tag{4.5}$$

and $v_j=(1+z_j^2)^{1/2}$. Note that for each $z_j \in (\pi j/\tilde{N}, \pi(j+1)/\tilde{N})$, with $j=1, 2,\ldots$, there is a single solution of (4.5), so that, for any $\tilde{N}$, $\tilde{M}>0$, convergence of the product

$$S(\tilde{M}, \tilde{N}) = s\text{-lim } T(M, N) = \prod_j \coth\left(\frac{\tilde{M}(1+z_j^2)}{4}\right)^{1/2} \tag{4.6}$$

is assured. Thus, we can construct a scaling limit from (2.32):

$$\mathscr{F}(\tilde{M}, \tilde{N}) = s\text{-lim } 2\xi_\perp \tau(\tilde{M}\xi_\perp, \tilde{N}\xi_{||}) = \frac{2}{\tilde{M}} \ln\left(\frac{S(\tilde{M}, \tilde{N})+1}{S(\tilde{M}, \tilde{N})-1}\right) \tag{4.7}$$

Notice that the critical coupling values only enter the results through $\xi_{||}$ and $\xi_\perp$, which, of course, are not required *a priori* to be equal.

We now examine various limits.

1. $\tilde{N}$ *large*: from (4.5), for $j \ll \tilde{N}$, we have $z_j = 2\pi j/\tilde{N}$, so (4.6) gives

$$S(\tilde{M}, \tilde{N}) \sim \prod_{j=1}^{\infty} \coth\left(\frac{\tilde{M}}{4}\left[1+\left(\frac{2\pi j}{\tilde{N}}\right)^2\right]^{1/2}\right) \tag{4.8}$$

which with $\tilde{M}$ large simplifies to

$$\begin{aligned} S(\tilde{M}, \tilde{N}) &\sim \exp\left\{\frac{\tilde{N}}{2\pi}\int_{-\infty}^{\infty} \exp\left[-\frac{\tilde{M}}{2}(1+x^2)^{1/2}\right]dx\right\} \\ &\sim 1+\frac{\tilde{N}}{(\pi\tilde{M})^{1/2}}\exp\left(\frac{-\tilde{M}}{2}\right) \end{aligned} \tag{4.9}$$

Inserting in (4.7) gives

$$\begin{aligned}\mathscr{F}(\tilde{M}, \tilde{N}) &\sim \frac{2}{\tilde{M}} \ln\left(\frac{2(\pi\tilde{M})^{1/2} e^{\tilde{M}/2}}{\tilde{N}}\right)\\ &= 1 + \frac{2}{\tilde{M}} \ln\left(\frac{\sqrt{\tilde{M}}}{\tilde{N}}\right) + O\left(\frac{1}{\tilde{M}}\right)\end{aligned} \tag{4.10}$$

2. $\tilde{N} \to 0$; we have $z_j \sim (2j+1)\pi/\tilde{N}$, for $j = 0, 1,...$; the condition $z_j \gg 1$ necessary for this approximation to (4.5) is assured by $\tilde{N} \to 0$. Equation (4.6) reduces to

$$S(\tilde{M}, \tilde{N}) = \prod_{n=0}^{\infty} \frac{1 + q^{2n+1}}{1 - q^{2n+1}} \tag{4.11}$$

where $q = \exp(-\pi\tilde{M}/2\tilde{N})$; here we make no restrictions on $\tilde{M}$ other that $\tilde{M} > 0$. This product can be evaluated exactly in certain cases, including $\tilde{M} = \tilde{N}$, as described in Appendix A. We note that

$$S(\tilde{N}, \tilde{N}) = (1 + \sqrt{2})^{1/2} + O(\tilde{N}) \tag{4.12}$$

from which

$$\mathscr{F}(\tilde{N}, \tilde{N}) \sim \frac{2}{\tilde{N}} \ln\left(\frac{(1+\sqrt{2})^{1/2} + 1}{(1+\sqrt{2})^{1/2} - 1}\right) + O(1) \tag{4.13}$$

as $\tilde{N} \to 0$. In Appendix A, we also consider the small-$\tilde{N}$ correction to this formula, obtaining

$$\mathscr{F}(\tilde{N}, \tilde{N}) = \frac{2}{\tilde{N}} \ln\left(\frac{(1+\sqrt{2})^{1/2} + 1}{(1+\sqrt{2})^{1/2} - 1}\right) + \frac{\sqrt{2}\,(1+\sqrt{2})^{1/2} \ln(1+\sqrt{2})}{\pi} + o(\tilde{N}) \tag{4.14}$$

This gives

$$\mathscr{F}(\tilde{N}, \tilde{N}) = 0.6164715 + \frac{3.05714184}{\tilde{N}} \tag{4.15}$$

Mon and Jasnow[3] used the scaling ansatz

$$\mathscr{F}(\tilde{N}, \tilde{N}) \sim 1 + \frac{B}{\tilde{N}} \tag{4.16}$$

with the numerical estimate of B to be $B = 2.58172$. The leading term is a good approximation for small $\tilde{N}$, but the large-$\tilde{N}$ behavior has to be modified: from (4.10),

$$\mathscr{F}(\tilde{N}, \tilde{N}) \sim 1 - \frac{\ln \tilde{N}}{\tilde{N}} + o\left(\frac{1}{\tilde{N}}\right) \tag{4.17}$$

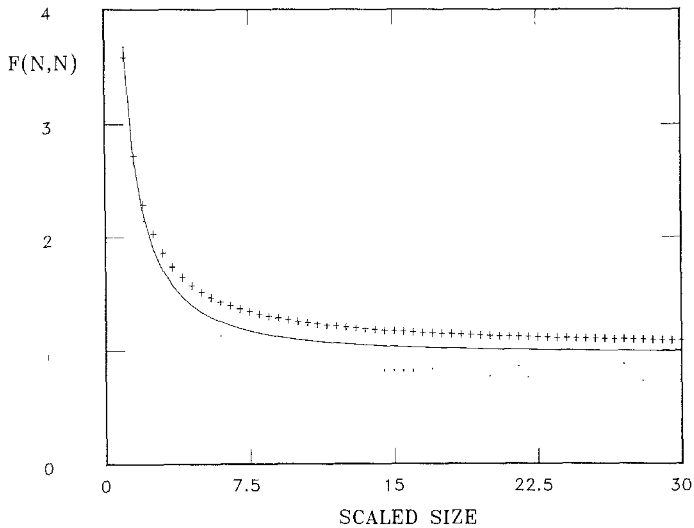

Fig. 1. Plot of the exact scaling function $\mathscr{F}(\tilde{N}, \tilde{N})$ vs. $\tilde{N}$ (full line), the Mon–Jasnow scaling ansatz (crosses), and the small-$\tilde{N}$ expansion (dots), obtained from (4.15). Also shown is the large-$\tilde{N}$ approximant (dots), for $\tilde{N} > 8$, Eq. (4.17).

We thank Fisher and Gelfand for pointing out a numerical error in ref. 7, which is corrected in (4.17); it is the coefficient of the $(\ln \tilde{N})/\tilde{N}$ term.

This term has an interesting origin, which we will analyze further in a later publication. Anticipating this, if we consider a transfer matrix around the cylinder, with fixed opposite spins at each end, then the capillary wave contribution arises precisely from the one-fermion sector.

The plot of the full scaling function from (4.7) and (4.6) is shown in Fig. 1. Also shown is the approximant (4.15), compared with the Mon–Jasnow scaling ansatz (4.16).

5. SUPERCRITICAL FINITE-SIZE EFFECTS

Returning to (3.3) and (3.4), it is clear that, when $T > T_c$, $B < 1$. This means that $\delta'(0) = 0$ [rather than $\delta'(0) = \pi$, which obtains for $T < T_c$] and that there is a real solution for e^{γ} given approximately by

$$e^{\gamma_0} = B + 2B^{2N} e^{2(K_2 - K_1^*)} (\cosh 2K_2^* - \cosh 2K_1) \sinh^2 2K_2 + O(B^{4N}) \tag{5.1}$$

which gives

$$v_0 = \kappa B^N + O(B^{2N}) \tag{5.2}$$

with

$$\kappa = 2 \sinh 2K_2 \,(\cosh 2K_2^* - \cosh 2K_1^*) \tag{5.3}$$

There are also unimodular solutions for e^{γ}, which behave much as those in the $T < T_c$ case and are therefore dominated in (3.12) by the real one, giving

$$T(M, N) \sim \frac{2}{M\kappa} B^{-N} \tag{5.4}$$

which diverges with N, giving

$$\tau(M, N) \sim \kappa B^{N} \tag{5.5}$$

There is a crossover scaling function around the critical point between the $T < T_c$ and $T > T_c$ regimes which can be obtained by scaling the lengths in (5.4) and adding in the contribution from the unimodular e^{γ}. We omit the details of this calculation.

APPENDIX A

In this Appendix we evaluate the infinite product

$$\mathscr{P}(q) = \prod_{0}^{\infty} \frac{1 + q^{2n+1}}{1 - q^{2n+1}} \tag{A.1}$$

by appealing to the theory of theta functions as discussed by Whittaker and Watson.[14] It is a standard result (found in connection with the spontaneous magnetization in Yang[15]) that

$$\mathscr{P}(q) = \left[\frac{\vartheta_3(0 \mid \tau)}{\vartheta_4(0 \mid \tau)}\right]^{1/2} \tag{A.2}$$

where $q = \exp(\pi i \tau)$ defines τ, and $\vartheta_j(z \mid \tau)$ are the standard theta functions.[16] It is also known that

$$\frac{\vartheta_3(0 \mid \tau)}{\vartheta_4(0 \mid \tau)} = \frac{1}{(1 - k^2)^{1/4}} \tag{A.3}$$

where k is the modulus of the complete elliptic integrals, which are related by

$$\frac{\mathscr{K}'(k)}{\mathscr{K}(k)} = -i\tau \tag{A.4}$$

This is a problem in the book by Whittaker and Watson.[14] In our case, with $\tilde{M}=\tilde{N}$, we have $q=\exp(-\pi/2)$, so that $\tau=i/2$. Thus we have to solve the equation

$$2\mathscr{K}'(k)=\mathscr{K}(k) \tag{A.5}$$

This is a particular example of a remarkable result of Abel,[14] which we quote without proof:

Theorem. Let

$$\frac{\mathscr{K}'(k)}{\mathscr{K}(k)}=\frac{a+b\sqrt{n}}{c+d\sqrt{n}} \tag{A.6}$$

where a, b, c, d, and n are integers. Then k is a root of an algebraic equation with integer coefficients. Equation (A.5) is obviously such an example. It turns out that $1-k^2=(\sqrt{2}-1)^4$. Using (A.3) and (A.2), the result (4.8) finally follows.

We now give a more refined estimate of the function $S(\tilde{M},\tilde{N})$. For small $\tilde{N}$, the roots of (4.5) are, up to $O(1)$ terms,

$$z_j=\frac{\pi(2j+1)}{\tilde{N}}+\frac{2}{\pi(2j+1)} \tag{A.7}$$

Inserting this in (4.6) gives

$$S(\tilde{M},\tilde{N})=\mathscr{P}(\lambda)\left\{1-\tilde{N}\sum_0^\infty \frac{2\lambda e^{-\lambda\pi(j+1/2)}}{\pi(2j+1)[1-e^{-2\lambda\pi(j+1/2)}]}\right\} \tag{A.8}$$

where $\lambda=\tilde{M}/\tilde{N}$. Consider the Fourier series

$$\operatorname{sn} u=\frac{2\pi}{\mathscr{K}k}\sum_0^\infty \frac{q^{n+1/2}}{1-q^{2n+1}}\frac{\sin(2n+1)\,\pi u}{2\mathscr{K}} \tag{A.9}$$

Integrating the right-hand side gives

$$\int_0^{\mathscr{K}} \operatorname{sn} u\,du=\frac{4}{k}\sum_0^\infty \frac{q^{n+1/2}}{1-q^{2n+1}}\frac{1}{2n+1} \tag{A.10}$$

from which we have

$$\sum_0^\infty \frac{q^{n+1/2}}{1-q^{n+1/2}}\frac{1}{n+1/2}=\frac{1}{4}\ln\left(\frac{1+k}{1-k}\right) \tag{A.11}$$

To make contact with (A.8), we put $q = e^{-\lambda\pi}$, which is not the same as that in the product analysis above. The parameter k in (A.11) is given by

$$\lambda = \frac{\mathscr{K}'(k)}{\mathscr{K}(k)} \tag{A.12}$$

For $\lambda = 1$, we have $k = 1/\sqrt{2}$, giving

$$\sum_0^\infty \frac{e^{-\pi(j+1/2)}}{1 - e^{-2\pi(j+1/2)}} \frac{1}{j+1/2} = \frac{1}{2} \ln(1 + \sqrt{2}) \tag{A.13}$$

Thus,

$$S(\tilde{N}, \tilde{N}) = \mathscr{P}(1) \left\{ 1 - \frac{\tilde{N}}{2\pi} \ln(1 + \sqrt{2}) \right\} \tag{A.14}$$

Inserting this in (4.7) gives

$$\mathscr{F}(\tilde{N}, \tilde{N}) = \frac{2}{\tilde{N}} \ln \left(\frac{\mathscr{P}(1) + 1}{\mathscr{P}(1) - 1} \right) + \frac{\sqrt{2}\, \mathscr{P}(1) \ln(1 + \sqrt{2})}{\pi} \tag{A.15}$$

with

$$\mathscr{P}(1) = (1 + \sqrt{2})^{1/2} \tag{A.16}$$

APPENDIX B

From (3.12), Taylor's theorem with remainder gives

$$\left| T(M, N) - 1 - 2 \sum_1^{N-1} e^{-Mv_j(N)} \right| \leqslant d \sum_1^{N-1} e^{-2Mv_j(N)} + f \left(\sum_1^{N-1} e^{-Mv_j(N)} \right)^2 \tag{B.1}$$

where d and f depend on $Mv_{\min}$ and are bounded whenever $Mv_{\min} > 0$.
We now examine (3.18), obtaining

$$\left| v_j(N) - 2(K_1 - K_2^*) - \frac{u}{2} \left(\frac{\pi j}{N} \right)^2 \right| \leqslant c \left(\frac{\pi j}{N} \right)^4 \tag{B.2}$$

provided $K_1 > K_2^*$ strictly, for some $c > 0$ uniformly in j. We have

$$\sum_1^{N-1} e^{-Mv_j(N)} = e^{-2M(K_1 - K_2^*)} Q(M, N) \tag{B.3}$$

where

$$Q(M, N) = \sum_{1}^{N-1} e^{-M(v_j(N) - v_j(\infty))} \tag{B.4}$$

Bringing in (B.2) and (3.18) gives

$$\left| Q(M, \alpha M^{1/2}) - \sum_{1}^{\alpha M^{1/2}} \exp\left[-\frac{u}{2}\left(\frac{\pi j}{\alpha}\right)^2 \right] \right| \leqslant \frac{g}{M} \sum_{1}^{\infty} \left(\frac{\pi j}{\alpha}\right)^4 \exp\left[-\frac{u}{2}\left(\frac{\pi j}{\alpha}\right)^2 \right] \tag{B.5}$$

for $\alpha > 0$ and some $g > 0$, again by Taylor's theorem with remainder. Finally, we have

$$\left| Q(M, \alpha M^{1/2}) - \sum_{1}^{\infty} \exp\left[-\frac{u}{2}\left(\frac{\pi j}{\alpha}\right)^2 \right] \right| \leqslant \frac{h}{M} + \int_{\alpha M^{1/2}}^{\infty} dx \exp\left[-\frac{u}{2}\left(\frac{\pi x}{\alpha}\right)^2 \right] \tag{B.6}$$

from which Result 2 [Eq. (3.16)] follows immediately.

APPENDIX C: CALCULATION OF Z^{+-}

For canonical transformations the identity

$$F^{\dagger}_{-\omega} F^{\dagger}_{\omega} + F_{\omega} F_{-\omega} = G^{\dagger}_{-\omega} G^{\dagger}_{\omega} + G_{\omega} G_{-\omega} \tag{C.1}$$

is easily established.

Let us define

$$U_{+}(\theta) = \exp i \sum \theta_{\omega} (F^{\dagger}_{-\omega} F^{\dagger}_{\omega} + F_{\omega} F_{-\omega}) \tag{C.2}$$

where the sum is on $\omega \in (0, \pi]$ such that $\exp(iM\omega) = -1$ (we take M even). Then

$$|\Phi^0_{+}\rangle = U_{+}(\theta_0)\, |0\rangle = U_{+}(-\delta^*/2)\, |\Phi_{+}\rangle \tag{C.3}$$

using $\delta^* = 2(\theta - \theta_0)$ and an obvious group property. Expanding $U_{+}(-\delta^*/2)$ using (C.1) and the vacuum property $G_{\omega} |\Phi_{+}\rangle = 0$, with $\exp(iM\omega) = -1$, gives

$$|\Phi^0_{+}\rangle = \prod_{>0}^{<\pi} \left(\cos\frac{\delta^*}{2} - i \sin\frac{\delta^*}{2}\, G^{\dagger}_{-\omega} G^{\dagger}_{\omega} \right) |\Phi_{+}\rangle \tag{C.4}$$

from which (2.26) and (2.29) follow directly.

Since M is even, $\omega = \pi$ satisfies $\exp(iM\omega) = 1$. Equation (2.27) follows from the analogue of (C.4) in this case.

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