Exact Finite-Size Effects in Surface Tension

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Exact finite-size effects for the interfacial free energy of the planar Ising ferromagnet are obtained. They are compared with a scaling function estimated by Mon and Jasnow using Monte Carlo simulation.

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The theory of finite-size scaling[1] and of finite-size effects in general has recently received new impetus from two sources. First, it is becoming clear that Monte Carlo simulations can only be useful for estimating thermodynamic limiting quantities when furnished with proper extrapolation procedures.[2] This means the fitting of parameters in some assumed finite-size form which preferably has a theoretical justification. Another use is in finite-dimensional transfer matrix methods, which enable one to calculate quantities in a strip of finite width but infinite length. Extrapolation is then made over matrix dimension.

This Letter presents new results for finite-size effects in the surface tension, denoted τ (also called the interfacial free energy), for the Ising model. This investigation was stimulated by recent work of Jasnow and Mon,[3-5] who addressed the amplitude relation

$$\tau_0 \xi_0^{d-1} = \text{const}, \tag{1}$$

where the surface tension behaves in the critical region as $\tau \sim \tau_0 t^{\mu}$ with $t=(T_c-T)/T_c$ and the correlation length ξ behaves as $\xi \sim \xi_0 t^{-\nu}$. The indices are related by Widom scaling $(d-1)\nu=\mu$.[6] Equation (1) is rigorous for $d=2$ provided a little care is used in the definition of ξ[7]; this follows from duality. For $d=3$, the dual model is the ferromagnetic plaquette one; dimensional scaling and universality have to be involved to justify (1).[7]

At present, experimental work for $d=3$ on (1), reviewed by Moldover,[8] shows a 30% or so discrepancy from best theoretical estimates; these were obtained from Monte Carlo data which is bedeviled by finite-size and by finite-time effects. If the surface tension is written as

$$\tau = \tau_0 t^{\mu} \Sigma(L t^{+\nu}), \tag{2}$$

in the usual scaling *Ansatz*, then for $d=2$ Mon and Jasnow used the form (which we show below to be an approximate one)

$$F(x) = 1 + B/x, \tag{3}$$

with $\mu=\nu=1$ to get τ_0 and B.

The agreement of τ_0 with exact results[9-11] for $d=2$ is satisfactory, lending confidence in the $d=3$ work. It has been known for some time that many different definitions of surface tension give the same result for $d=2$.[12] In the present work we evaluate $F(x)$ in (2) exactly for the geometry used by Mon and Jasnow[3]; we shall show elsewhere that $F(x)$ depends markedly on the type of definition used for τ; floating interfaces and ones pinned at the ends have quite different forms for $F(x)$.

We consider a square lattice wrapped on a cylinder of height N and circumference M with coupling K_1 parallel to the axis and K_2 in the other direction. Phase separation is induced by the imposition of boundary conditions $\mathscr{B}$ on the faces of the cylinder (i.e., otherwise free edges of the lattice): If the spin variables $\sigma(i)$ have the value $+1$ on the top and -1 on the bottom, denoted $\mathscr{B}=+-$, then there must be an odd number of domain walls running around the cylinder, whereas if $\sigma(i)=+1$ on both top and bottom, denoted $\mathscr{B}=+$, then there will be an even number of such walls. Provided the thermodynamic limit is taken with M/N fixed, $M\to\infty$ and $N\to\infty$, then for low enough temperatures it is conjectured with $\mathscr{B}=+-$ ($\mathscr{B}=+$) with probability one there is exactly one (exactly no) such domain wall.[11,13,14]

Thus the proper definition of surface tension is

$$\tau = \lim \tau(M,N),$$

where

$$\tau(M,N) = -M^{-1}\ln(Z^{+-}/Z^{+}), \tag{4}$$

$Z(\mathscr{B})$ being the canonical partition function for boundary condition $\mathscr{B}$. This has been evaluated exactly[15] for any M and N, giving

$$Z^{+-}/Z^{+} = [T(M,N)-1]/[T(M,N)+1], \tag{5}$$

with

$$T(M,N) = \exp \textstyle\sum_j \ln \coth[\tfrac{1}{2} M v_j(N)], \tag{6}$$

where $v_j(N) > 0$ and

$$\cosh v_j = \cosh 2(K_1 - K_2^*) + \sinh 2K_1 \sinh 2K_2^* (1-\cos t_j) \qquad (7)$$

with the t_j solutions of

$$e^{iNt} = \pm \left(\frac{1}{AB}\right)^{1/2} \left(\frac{(e^{it}-A)(e^{it}-B)}{(e^{it}-A^{-1})(e^{it}-B^{-1})}\right)^{1/2}, \qquad (8)$$

where $\exp(2K_j^*) = \coth K_j$, $j=1,2$, and $A = \exp[2(K_1 + K_2^*)]$, $B = \exp[2(K_1 - K_2^*)]$. The root $t=0$ of (8) is not allowed. Provided $v_0 > 0$, where $v_0 = 2(K_1 - K_2^*)$ is the surface tension for the infinite system, the roots are

$$v_j = v_0 + u_0(\pi j/N)^2 + O(1/N^4) \qquad (9)$$

for $j=1, \ldots$ with

$$u_0^{-1} = 2\sinh 2K_1^* \sinh 2K_2 \sinh v_0.$$

At $T = T_c$, $v_0 = 0$ and

$$v_j = \pi(2j-1)/(2N+1) + O(1/N^2). \qquad (10)$$

It follows from (9) that for $v_0 > 0$ (i.e., $T < T_c$),

$$\lim_{M\to\infty} \tau(M,N) = v_0 + u_0(\pi/N)^2 + O(1/N^4). \qquad (11)$$

The fluctuations of the domain wall are restricted by the finite geometry, giving an entropic repulsion as advocated by Fisher and Fisher[16] in a random-walker or solid-on-solid model of the interface.

It is known that an interface of length M pinned at its ends fluctuates on a length scale of $M^{1/2}$.[17] With the cylindrical boundary conditions we would expect a crossover phenomenon in terms of the variable $\alpha = N/M^{1/2}$. It follows from (5) to (8) that

$$\lim_{M\to\infty} M\{\tau(M,\alpha M^{1/2}) - v_0\} = -\ln \sum_1^\infty \exp[-u_0(\pi j/\alpha)^2]. \qquad (12)$$

The asymptotic behavior is $\sim u_0\pi^2/2\alpha^2$ as $\alpha \to 0$ leading back to (11), whereas as $\alpha \to \infty$ the behavior is $\sim -\ln\alpha$.

The previous set of results should be typical (at least at low enough temperatures *stricto sensu*) of ensembles with one and no domain wall running around the cylinder.[9,14] If we take $N = \exp(\lambda M)$ we anticipate configurations with many domain walls, depending on λ:

$$\lim_{M\to\infty} \tau(M, e^{\lambda M}) = 0 \quad \text{if } \lambda \geqslant v_0$$
$$= -\lambda + v_0 \quad \text{if } 0 \leqslant \lambda \leqslant v_0. \qquad (13)$$

This result can be understood as follows. The entropy of a "gas" of n domain walls on the cylinder is composed of two parts: There is the *flexural* entropy of a domain wall in isolation, included in the incremental free energy $2(K_1 - K_2^*)$ of a domain wall in isolation. Then there is the entropy of the domain walls treated as one-dimensional fermions on a line of length N. This separation is, of course, an approximation but a free-energy minimization gives the first part of (13) for $\lambda > v_0$; there is an infinite number of domain walls as $M \to \infty$ so that there is no essential difference between $\mathscr{B}_{+-}$ and $\mathscr{B}_{+}$. The potential proliferation of domain walls was anticipated by Fisher, Barber, and Jasnow[18] and placed on a more precise footing by Privman and Fisher[19] and by Brézin and Zinn-Justin.[20] The result (13) is rigorous.

Finally we consider the finite-size scaling problem, as suggested in (2). Following the Privman-Fisher hypothesis,[21] we would expect (2) to be written as

$$\tau \sim L^{-1} f(c_1 t l), \qquad (14)$$

where L is the system size, c_1 is nonuniversal [depending on $K_1(c)$ and $K_2(c)$], and $f(y)$ depends on the *shape* of the lattice and on the particular definition used for τ. The last point will be explored elsewhere. The dependence on the couplings comes out nicely as follows: From the basic Widom scaling idea, we expect $\tau\xi_2 \sim \frac{1}{2}$ in units of kT where ξ_2 is the correlation length in the direction of K_2. Wu[22] showed that

$$\xi_1^{-1} = 4(K_2 - K_1^*)$$

and

$$\xi_2^{-1} 4(K_1 - K_2^*)$$

(notice the low-temperature anomalous factors of 2). Define the scaled lengths by $(M, N \to \infty,\ t \to 0)$

$$s - \lim M/\xi_2 = \tilde{M}, \quad s - \lim N/\xi_1 = \tilde{N}. \qquad (15)$$

Then

$$s - \lim(2\tau\xi_2) = F(\tilde{M},\tilde{N}), \qquad (16)$$

where

$$F(\tilde{M},\tilde{N}) = \frac{1}{\tilde{M}} \ln \frac{S(\tilde{M},\tilde{N})+1}{S(\tilde{M},\tilde{N})-1}, \qquad (17)$$

with

$$S(\tilde{M},\tilde{N}) = \exp \sum_j \ln \coth[\tfrac{1}{2}\tilde{M}(1+z_j^2)^{1/2}], \qquad (18)$$

where

$$\tan \tilde{N} z_j \sim -\tilde{N}. \qquad (19)$$

The dependence on $K_1(c)$ and $K_2(c)$ is contained entirely within $\tilde{M}$ and $\tilde{N}$. As $\tilde{M}$ and $\tilde{N} \to \infty$,

$$S(\tilde{M},\tilde{N}) \sim \exp[2\tilde{N}(2\pi\tilde{M})^{-1/2} e^{-\tilde{M}}],$$

so that if the argument of exp is small,[17,18]

$$s-\lim(2\tau\xi_2) \sim 1-\frac{1}{\tilde{M}}\{\ln(\tilde{N}/\sqrt{\tilde{M}})+O(1)\}. \quad (20)$$

This implies that the Mon-Jasnow *Ansatz* is not exact (but it seems very good numerically). The behavior for small $\tilde{M},\tilde{N}$ is given by

$$S(\tilde{M},\tilde{N})\sim\prod_0^{\infty}\frac{1+q^{2n+1}}{1-q^{2n+1}}, \quad (21)$$

where

$$q=\exp(-\tfrac{1}{2}\pi\tilde{M}/\tilde{N}).$$

The reader familiar with theta functions should find that if $\tilde{M}=\tilde{N}$, then

$$\lim_{\tilde{M}\to 0} S(\tilde{M},\tilde{N})=(1+\sqrt{2})^{1/2}. \quad (22)$$

Returning to the Mon-Jasnow function

$$\Sigma(Mt)\sim 1+B/Mt$$

we find $B_{\text{exact}}\sim 0.868\,370\,8$ to be compared with the Monte Carlo estimate $B_{\text{MC}}\sim 0.7323$.

The dependence of the finite-size scaling function on size ratio and on $K_1(c)$ and $K_2(c)$ is thus more complicated than in (14) *et. seq.*

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