Finite-Size Properties of the Angle-Dependent Surface Tension of Rough Interfaces

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A study is reported of finite-size, L, corrections for the surface tension of rough interfaces, i.e., for temperatures $T_R < T < T_c$ in 3D, $0 < T < T_c$ in 2D. A universal leading contribution proportional to $(\ln L)/L$ is predicted in 2D. This term is a result of the characteristic rough interface fluctuations. In 3D, the leading corrections are of order $1/L$.

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Recent Monte Carlo (MC) studies[1] of the roughening transition and related interfacial properties in the 3D Ising model have raised an interesting theoretical question regarding the finite-size effects on the anisotropic surface tension of rough interfaces. To define the problem, consider first for simplicity a 2D Ising-like system of size $L\times M$, depicted in Fig. 1. By the fixing of the boundary spins as shown, an interface is induced connecting the points (0,0) and (L,h). Note that $T<T_c$ is assumed, and I suppress the parametric T dependence of various quantities.

Let $Z(h,L;M)=Z_{+-}/Z_{++}$ denote the partition function of the system normalized by the partition function of a reference *single-phase* system obtained by the replacement of all the fixed negative boundary spins by positive ones. For *fixed h*, with L and M large, let us define the step free energy in 2D by

$$s(h,L;M)=-\ln[Z(h,L;M)/Z(0,L;M)], \quad (1)$$

where we measure all the free energies in units of k_BT.

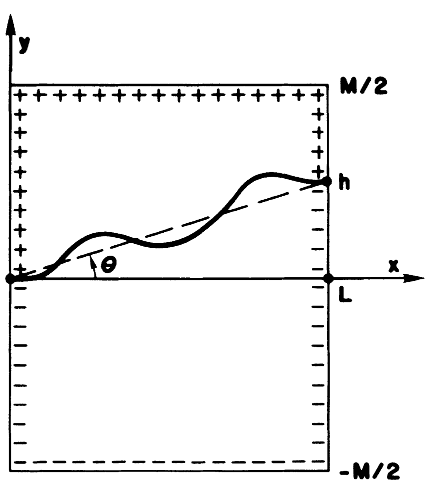

FIG. 1. Finite-size 2D Ising-type system of dimensions $L\times M$. (For symmetry, I take M even.) A long contour separating the regions of opposite magnetizations is shown schematically.

If, however, we fix the angle by requiring $h=L\tan\theta$ (see Fig. 1), we can define the surface tension in 2D, per unit length (and per k_BT),

$$\sigma(\theta,L;M)=-(\cos\theta/L)\ln Z(L\tan\theta,L;M). \quad (2)$$

My aim is to analyze finite-L (and M, etc.) effects for rough, i.e., strongly fluctuating, interfaces. Thus, we can choose any T from $0<T<T_c$ in 2D, but $T_R<T<T_c$ in 3D (see van Beijeren and Nolden[2]); the precise definition of sizes, s,σ, in 3D will be given later. I consider the case when the x axis (Fig. 1) coincides with a symmetry direction of the underlying lattice structure, and assume a local stable minimum of $\sigma(\theta)/\cos\theta$ (i.e., free energy per unit *projected* length). For the bulk $(L,M=\infty)$ quantities we have $s(h,\infty;\infty)=0$, and

$$\sigma(\theta,\infty;\infty)/\cos\theta=\tau+\tfrac{1}{2}\kappa\theta^2+O(\theta^4), \quad (3)$$

with

$$\tau\equiv\sigma(0,\infty;\infty)>0,$$
$$\kappa\equiv\sigma(0,\infty;\infty)+\sigma''(0,\infty;\infty)>0. \quad (4)$$

I always assume $M=O(L)$, and $|h|\ll L$, which corresponds to $|\theta|\ll 1$ in (2).

Studies of finite-size effects on interfacial properties have been initiated in recent years. Several regimes of interest can be identified. For $T\simeq T_c^-$, a finite-size scaling description has been formulated for the surface tension[3,4] with an emphasis on universal amplitudes,[3-5] similar to the bulk quantities.[6] Near T_R, scaling forms have been conjectured[1,7] and tested by numerical MC[1] and transfer-matrix[7] calculations. A related topic of finite-size scaling at wetting transitions has been investigated recently.[8,9]

Away from the "critical" regions near T_c and T_R, for $T_R<T<T_c$ (with $T_R=0$ in 2D), one can consider size effects on the fluctuations of rough interfaces. For a linear interface of length L in 2D (Fig. 1), the transverse fluctuations[2,10] are on the y scale $\sim\sqrt{L}$. (The analogous scale in 3D is $\sim\ln L$.) If the transverse system size, M, is of order $\sqrt{L}$ or less (in 2D), then the interface fluctuations will be suppressed: Such effects have been exten-

sively studied for 2D systems.[8,10-12] Available results in 3D are more limited.[10] Since we consider $M=O(L)$, the finite-M effects are exponentially small in $M^2/L \sim L$. Thus, I will omit the M dependence of various quantities below.

My study of finite-L effects will be formulated first for the 2D case. Extension to 3D will follow. My main results are represented by relations (8) and (9) and (18) and (19) below. Relevant MC[1] and exact[13,14] results available in the literature will be discussed; however, I also checked my 2D predictions by extensive solid-on-solid model calculations.[14] Finally, the case of the "rigid" interfaces for $T<T_R$ (in 3D) is outside the scope of the present investigation.

It is well established (see Fisher[15] for a review) that the probability distribution for a contour separating the $\pm$ regions (Fig. 1) to reach a height $h=L\tan\theta \simeq L\theta$ at a distance L along a symmetric lattice direction is Gaussian in h, for $|h| \ll L$, with width $\sim\sqrt{L}$. This directed random-walk-like property of line interfaces in 2D has found extensive theoretical uses.[13,15] For the geometry of Fig. 1 we thus propose the following phenomenological expression for the partition function,

$$Z(L\theta,L) \simeq e^{-\tau_L L}(\kappa_L \lambda^2/2\pi L)^{1/2} e^{-\kappa_L L\theta^2/2}, \qquad (5)$$

valid for $|\theta| \ll 1$. The first factor models the free-energy cost of creation of an interface of length L. Thus, we expect $\lim_{L\to\infty}\tau_L=\tau$ [see (4)]. The last factor represents additional entropic effects due to interface inclination, measured with respect to $\theta=0$. The stiffness coefficient in the bulk limit is κ (see Fisher and coworkers.[16,17]) Thus, $\lim_{L\to\infty}\kappa_L=\kappa$. The *normalization factor* in (5) has been calculated in terms of the dimensionless displacement $h/\lambda \simeq L\theta/\lambda$, where λ is a microscopic length scale of the order of one lattice spacing, by my first rewriting the Gaussian factor as $\exp[-(\kappa_L\lambda^2/2L)(h/\lambda)^2]$. Less "microscopic" arguments substantiating relation (5), which can also be extended to the 3D case, will be proposed later.

The quantities τ_L and κ_L are noncritical. We therefore expect standard $O(L^{-1})$ "end-point" finite-size corrections.[18] Thus, I conjecture

$$\tau_L=\tau+a/L+o(L^{-1}), \quad \kappa_L=\kappa+b/L+o(L^{-1}). \qquad (6)$$

Recall that a, b, and other "constants" are T dependent.

Since relation (5) should be accurate up to corrections of order $L\theta^4$ additive to $L\theta^2$ in the exponential, it can only be used to estimate the first two terms in the expansion

$$\sigma(\theta,L)=\sigma(0,L)+\tfrac{1}{2}\sigma''(0,L)\theta^2+O(\theta^4). \qquad (7)$$

By using (2), we get

$$\sigma(0,L)=\sigma(0,\infty)+\frac{\ln(L/\lambda)}{2L}+\frac{a-\ln(\lambda\kappa/2\pi)^{1/2}}{L}+o\left(\frac{1}{L}\right), \qquad (8)$$

$$\sigma''(0,L)=\sigma''(0,\infty)-\frac{\ln(L/\lambda)}{2L}+\frac{b-a+\ln(\lambda\kappa/2\pi)^{1/2}}{L}+o\left(\frac{1}{L}\right). \qquad (9)$$

Note that the leading correction terms, $\pm(\ln L)/2L$, have no free parameters. Although no detailed study has been published for the 2D Ising model in the geometry considered here, Abraham[13] reported the presence of the $(\ln L)/2L$ correction in $\sigma(0,L)$, which he found "surprising" (see pp. 63 and 64 of Ref. 13). For solid-on-solid model results, consult Ref. 14.

For the step free energy (1), we use (5) with h fixed. The discreteness of small angles $\theta \simeq h/L$, corresponding to h of the order of few lattice spacings, is not significant. Indeed, the Gaussian distribution in h is a central-limit-theorem-type result and only requires $|h| \ll L$. We get

$$s(h,L) \simeq \kappa h^2/2L. \qquad (10)$$

This relation was derived (for 2D and 3D, with a somewhat different notation) by Fisher and Weeks,[17] within the capillary-wave theory.[19,20] The interface is described by a smooth *single-valued* function $y(x)$; compare Fig. 1. The free energy of small distortions is modeled by $\frac{1}{2}\kappa\int_0^L dx[y'(x)]^2$. The effect of a step is estimated[17] by the replacement of $y'(x)$ by the average interface slope h/L. Such a mean-field-type estimate should be correct at this coarse-grained level of description, with the "macroscopic" κ. Indeed, (10) is obtained. Note the characteristic $1/L$ and h^2 dependences. Relations (8)-(10) have been confirmed by explicit 2D solid-on-solid model calculations.[14]

For an interface of length l, forming a *small* angle ϕ with symmetric direction, we can calculate the angle-dependent step free energy $s_\phi(h,l)$ by using relation (5). Thus, the reference interface connects the origin of the xy plane to the point $(l\cos\phi, l\sin\phi)$, while the "stepped" interface ends at a point displaced perpendicularly by h, i.e., at $x=l\cos\phi-h\sin\phi$, $y=l\sin\phi+h\cos\phi$. For $|\phi| \ll 1$, a long calculation yields

$$s_\phi(h,l)=\sigma''(0,\infty)h\phi+h[2h\kappa+2(2b-1)\phi+3h\kappa\phi^2]/4l+o(l^{-1},\phi^2). \qquad (11)$$

The leading correction ($\sim 1/l$) shows the crossover to (10) as $\phi \to 0$.

In 3D, we introduce the third coordinate axis, z, pointing out of the plane of Fig. 1. We consider a finite system of size $L\times M\times N$, with $0\leq z\leq N$, where $N=O(L)$. The boundary conditions at the $x=0,L$ and $y=\pm M/2$ faces are shown in Fig. 1, for $z=0$. They are extended identically for all $0\leq z\leq N$. At the $z=0,N$ faces, we assume free boundary conditions. Thus the interface is perpendicular to the xy plane and forms an angle θ with the xz plane. Generally, the orientation of interfaces in 3D, with respect to a reference plane (xz here), is specified by *two angles*. We assume that xz is a symmetry plane such that the surface tension measured per unit *projected* area (in the xz plane), σ_P, has a local minimum when the interface is in the xz plane, as compared to *all* inclinations.

Let $\bar{x}y\bar{z}$ denote a coordinate system obtained by a rotation by angle γ about the y axis. We specify the inclination of a general plane by the angles α and β formed by the intersection of the $\bar{x}y$ and $y\bar{z}$ planes with the $\bar{x}$ and $\bar{z}$ axes, respectively. The quantities $\sin\alpha$ and $\sin\beta$ undergo orthogonal transformations upon y rotations. Thus one can find an appropriate γ with a *principal* coordinate system such that the minimum of $\sigma_P(\alpha,\beta)$ is diagonal, for small α and β,

$$\sigma_P(\alpha,\beta)\simeq\tau+\tfrac{1}{2}\kappa_1\alpha^2+\tfrac{1}{2}\kappa_2\beta^2, \tag{12}$$

with $\tau,\kappa_1,\kappa_2>0$; compare (3) and (4). However, in order to avoid unilluminating mathematic complications, we will use a one-angle description. This corresponds to interfaces with the normal vector in the xy plane. The appropriate restriction for the α,β variables reads $\sin\beta/\sin\alpha=\tan\gamma$. The 3D surface tension is then defined by

$$\sigma(\theta,L,N;M)=-\frac{\cos\theta}{LN}\ln Z(h=L\tan\theta,L,N;M). \tag{13}$$

Relations with the forms (3) and (4) apply, with the effective stiffness coefficient given by

$$\kappa=\kappa_1\cos^2\gamma+\kappa_2\sin^2\gamma. \tag{14}$$

Other inclinations can, in principle, be accommodated by the redefinition (rotation) of the coordinate system, *and the $L\times M\times N$ sample boundaries*, about the y axis.

We are interested in a relation of the type (5). To this end, observe that the leading exponential dependencies in (5) can be obtained by the following phenomenological argument which we formulate here in the 3D notation. First, we solve (13) for Z. We then argue that for large L, $\sigma(\theta,L,N)/\cos\theta$ is well approximated by the bulk expansion (3) and (4). Therefore, for small θ, Z must have a leading exponential size dependence of the form $Z\sim\exp[-LN(\tau+\frac{1}{2}\kappa\theta^2)]$. The next step is to interpret this approximate equality by the identification of possible sources of finite-size corrections. A plausible conjecture is

$$Z(\theta,L,N)\simeq R(L,N)\exp[-LN(\tau_{L,N}+\tfrac{1}{2}\kappa_{L,N}\theta^2)], \tag{15}$$

where for the coefficients in the exponential we generally assume the leading 1/(size) corrections,[18]

$$\tau_{L,N}\simeq\tau+a/L+A/N,\quad \kappa_{L,N}\simeq\kappa+b/L+B/N. \tag{16}$$

The prefactor $R(L,N)$ accounts for possible power-law (in L,N) terms similar to the normalization factor $\sim 1\sqrt{L}$ in (5). However, with no "microscopic" substantiation of relation (15) available in 3D, it is not clear how to normalize the distribution in θ, or more generally, in the angles α,β. For example, if we *speculate* that a one-variable normalization in terms of dimensionless displacement $h/\lambda\simeq L\theta/\lambda$ suffices, we get

$$R(L,N)\propto(N/L)^{1/2}. \tag{17}$$

Fortunately, as long as R obeys a power law in L,N, the contribution due to this factor in 3D is not the leading one. Accepting (17) as a tentative estimate, we get

$$\sigma(0,L,N)\simeq\sigma(0,\infty,\infty)+a/L+A/N, \tag{18}$$

$$\sigma''(0,L,N)\simeq\sigma''(0,\infty,\infty)+\frac{b-a}{L}+\frac{B-A}{N}, \tag{19}$$

where the higher-order corrections in (18) and (19) are of order L^{-2} [recall that we assume $N=O(L)$], including terms $\pm\ln(L/N)/2LN$ due to the factor (17).

The form of (17) is suggestive of a more general conclusion. Indeed, when expressed in terms of the reduced displacement h/λ, the Gaussian dependence in (15) corresponds to the distribution width $\sim(L/N)^{1/2}\sim 1$. Even without the precise microscopic prescription for calculating the normalization factor R in 3D, we can anticipate a much weaker size dependence than in 2D, due to weaker interface fluctuations.

The 3D result[17] for the step free energy also follows, similarly to (10),

$$s(h,L,N;M)\equiv-\frac{1}{N}\ln\left[\frac{Z(h)}{Z(0)}\right]\simeq\frac{\kappa h^2}{2L}. \tag{20}$$

For the step free energy of a slightly inclined interface (but still perpendicular to the xy plane) the 3D analog of (11) reads

$$s_\phi(h,l,N)\simeq\sigma''(0,\infty,\infty)h\phi+h(2h\kappa+4b\phi+3h\kappa\phi^2)/4l+(B-A)h\phi/N, \tag{21}$$

where the notation was explained in connection with (11). As mentioned, relation (20) arises naturally[17] within the capillary-wave approach.[19,20] Note that (20) and (21) are not sensitive to the precise power-law dependences of $R(L,N)$, to the leading orders shown.

The $1/N$ correction term included in (16), (18), (19), and (21) can be eliminated[18] [finite-N effects in (16) made exponentially small] by use of periodic boundary conditions in the z direction. In the recent MC simulation[1] of the 3D Ising model of size $L \times L \times L$, the boundary conditions were periodic in z, antiperiodic in y, and helical in x; see Ref. 1 for details. Some $1/L$ surface-tension corrections are apparently present[1] even with these optimal boundary conditions, probably these are a/L and b/L type terms; see (18) and (19). The $1/L$ dependence of the step free energy (20) [which is *not* a result of corrections in (16)] has also been observed numerically.[1]

In summary, I have obtained new results[21] on the finite-size properties of the surface tension in 2D and 3D systems in the block geometry, for $T_R < T < T_c$. My 2D predictions are summarized by relations (8) and (9). A notable result is the universal form of the leading surface-tension correction in (8) and (9). The 3D results (18) and (19) are consistent with the recent MC findings.[1]

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[1]K. K. Mon, S. Wansleben, D. P. Landau, and K. Binder, Phys. Rev. Lett. **60**, 708 (1988).

[2]H. van Beijeren and I. Nolden, "The Roughening Transition" (unpublished).

[3]K. K. Mon and D. Jasnow, Phys. Rev. A **31**, 4008 (1985).

[4]D. B. Abraham and N. M. Švrakić, Phys. Rev. Lett. **56**, 1172 (1986).

[5]H. Park and M. den Nijs, unpublished.

[6]V. Privman and M. E. Fisher, Phys. Rev. B **30**, 322 (1984).

[7]J. M. Luck, J. Phys. (Paris), Lett. **42**, L277 (1981).

[8]V. Privman and N. M. Švrakić, Phys. Rev. B **37**, 3713 (1988).

[9]G. Forgacs, N. M. Švrakić, and V. Privman, Phys. Rev. B **37**, 3818 (1988).

[10]J. Bricmont, A. El Mellouki, and J. Fröhlich, J. Stat. Phys. **42**, 743 (1986).

[11]M. E. Fisher and D. S. Fisher, Phys. Rev. B **25**, 3192 (1982).

[12]J. Stecki and J. Dudowicz, Proc. Roy. Soc. London A **400**, 263 (1985).

[13]D. B. Abraham, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1986), Vol. 10, p. 1.

[14]Some solid-on-solid model results, including the leading finite-size correction, follow straightforwardly from the analysis by H. Park, E. K. Riedel, and M. den Nijs, Ann. Phys. (N.Y.) **172**, 419 (1986), Appendix B. A more detailed study, by N. M. Švrakić, V. Privman, and D. B. Abraham (to be published), confirms the conjectured expansion (6).

[15]M. E. Fisher, J. Stat. Phys. **34**, 667 (1984).

[16]M. P. A. Fisher, D. S. Fisher, and J. D. Weeks, Phys. Rev. Lett. **48**, 368 (1982).

[17]D. S. Fisher and J. D. Weeks, Phys. Rev. Lett. **50**, 1077 (1983).

[18]I follow lines of argument similar to those used to assess finite-size corrections to bulk quantities away from T_c. See M. E. Fisher, in *Critical Phenomena,* International School of Physics "Enrico Fermi," Course 51, edited by M. S. Green (Academic, New York, 1971), p. 1.

[19]F. P. Buff, R. A. Lovett, and F. H. Stillinger, Jr., Phys. Rev. Lett. **15**, 621 (1965).

[20]J. D. Weeks, J. Chem. Phys. **67**, 3106 (1977).

[21]After completing this work, I learned that M. E. Fisher and M. P. Gelfand have been developing a microscopic theory of finite-size effects on the surface tension for general D, within the capillary-wave–type approach originated by R. F. Kayser, Phys. Rev. A **33**, 1948 (1986). Wherever comparison is possible, their results are consistent with mine and with the solid-on-solid model conclusions (Ref. 14). The author thanks M. E. Fisher and M. P. Gelfand for communicating their results (which have been announced at the December 1987 Statistical Mechanics Meeting at Rutgers University, and at the June 1988 National Bureau of Standards Thermophysical Properties conference).