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# Finite-Size Scaling of the Interfacial Tension

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The interfacial free energy appropriate to a finite system in the Ising universality class is calculated to one-loop order. Consideration is given to the behavior in both three and four dimensions via an epsilon expansion. The results corresponding to three dimensions are compared with the simulation data of Mon and Jasnow.

**KEY WORDS:** Finite-size scaling; surface tension; renormalization group; collective coordinates.

## 1. INTRODUCTION

The critical properties of finite-size systems have attracted the attention of researchers ever since the original investigations of Fisher[1] in 1970. Of substantial importance was the discovery[2, 3] that the same field-theoretic techniques used in the description of critical bulk phenomena can also be applied to finite systems. In particular, it is possible to utilize the renormalization group and epsilon expansion to calculate finite-size scaling functions explicitly. However, at the present time there does not exist a field-theoretic analysis of the scaling function for the interfacial free energy associated with two phases in coexistence. An analysis of this type, while of interest in its own right, would also contribute to the body of literature that deals with systems lacking translational invariance. Furthermore, one is in the fortunate position of having accessible the results of numerical simulations[4, 5] with which to compare an analytical calculation.

Van der Waals[6] was perhaps the first to investigate theoretically the liquid–vapor interface. Almost a century later, when the universal behavior of systems near criticality had become a topic of great interest, Fisk and Widom[7] proposed a density functional approach in an attempt to modify the classical behavior characteristic of the van der Waals theory. Several

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years later when the revolutionary ideas of Wilson were being applied to various systems, two groups of researchers[8, 9] utilized these ideas to describe the interfacial profile of a critical liquid–vapor system. This represented the first application of the new renormalization group formalism to a spatially inhomogeneous system. Some ten years later, two groups of authors[10, 11] independently calculated the universal amplitude ratio $R_{\sigma\xi}$ involving the surface tension and correlation length amplitudes. However, it soon became apparent that while the theoretical estimates for the exponent $\mu$ were in respectable agreement with experiments and numerical simulations, this was not the case for the amplitude ratio $R_{\sigma\xi}$. The results of both an epsilon expansion and numerical simulation fell significantly short of the median value of $R_{\sigma\xi}$ for fluids, the former by 50%, and the latter by 30%, while two results were in agreement to within 20%. This state of affairs might have been reasonably interpreted as indicating the existence of a systematic error in the measurement of the surface tension. This, however, is now believed to be not the case. The discrepancy between the theoretical and experimental values is well outside of plausible systematic error.[12–14]

Somewhat recently, the discrepancies between the experiments and simulation data appear to have been resolved by Mon,[4] who has extracted information on the asymptotic form of the scaling function on substantially larger lattices than those used in prior simulations. The results of this and former simulations reveal that there is a very slow convergence of the scaling function onto its asymptotic form. Though the actual data of the simulation improve the estimate of the amplitude ratio, a method of extrapolation based on the presence of logarithmic subdominant terms to the scaling function improves the estimate further. Mon's use of such logarithmic terms to fit the data was based on analogy with the two-dimensional Ising model where such terms are known to be present. Given that the results of simulations and physical experiments are consistent, it appears that in this case the epsilon expansion is not as accurate as one might have expected. However, regarding this expectation, it should be kept in mind that the loop correction nearly *doubles* the mean field estimate of the amplitude ratio. As pointed out in refs. 15 and 16, large corrections like this are not uncommon for estimates of amplitude ratios. Consequently, such estimates often tend to be less reliable than the corresponding ones for exponents. In an attempt to overcome this problem, a fixed-dimension calculation of the amplitude ratio has recently been performed by Münster,[17] and yields a result which agrees with that of experiments to within a couple percent.

Of the relatively few direct comparisons between the results of renormalization group (RG)-based finite-size calculations[2, 3] and Monte Carlo

data, there is reasonable agreement.[3, 18] Part of the motivation for this article is to investigate to what extent the results of a field-theoretic analysis of the interfacial tension coincide with those of the numerical simulations. The program of making such comparisons is essential. Indeed, a Monte Carlo simulation can be viewed as an idealized, finite-sized experiment, which the field-theoretic method is challenged to describe. These types of calculations not only rely on standard methods found in bulk calculations, they also depend crucially on the nonperturbative treatment of coordinates. It is by no means obvious whether the rather novel methods that are used will faithfully reproduce quantitative results that are representative of the simulations. The comparison with simulation data thus serves as an ideal testing ground to assess whether the methods are yielding results in accord with our expectations. The present calculation, while proceeding in a manner similar to the previous analyses for uniform systems, is considerably more complex. The lack of translational invariance, while generally complicating matters mathematically, can even lead to problems in principle. Due to the broken translational invariance resulting from the interface, there is an additional degree of freedom that must be treated collectively. It also happens that the identification of the corresponding degree of freedom that arises in the uniform phase calculation is not only less clear, its collective treatment is more involved.

This article presents a calculation of the temperature and size dependence of the interfacial free energy for an Ising-like system in a finite volume to one-loop order near and at the bulk critical point. The approach taken is to adapt the methods developed by Brézin and Zinn-Justin[3] and Rudnick *et al.*[2] to a spatially inhomogeneous system. The results of the calculation are compared numerically with the three-dimensional simulation data of Mon and Jasnow.[4, 5] In particular, the interfacial free energy at the bulk critical point and the form of the subdominant corrections to the scaling function are considered. Also addressed is the behavior in four dimensions, where logarithmic corrections to the mean field behavior are expected. Because the behavior in four dimensions is generally not universal, it is only possible to present here results that should agree qualitatively with the Monte Carlo data. The results and discussion reported here may also provide simulators with a better sense of where they might expect to see signatures of logarithmic behavior, and aid them in the interpretation of their data.

Here I present some basic background on the surface tension. The surface tension, or interfacial free energy per unit area, vanishes as one approaches the critical point from below as

$$\sigma(t) \sim \sigma_0 |t|^{\mu} \tag{1.1}$$

where the exponent $\mu$ obeys the scaling relation

$$\mu = 2 - \alpha - \nu \tag{1.2}$$

or, if one invokes hyperscaling,

$$\mu = \nu(d-1) \tag{1.3}$$

For a finite system, if a finite-size scaling ansatz is assumed, the interfacial free energy $\Sigma$ and surface tension $\sigma$ take the form

$$\Sigma(t, L) = Y(atL^{1/\nu}) \tag{1.4}$$

$$\sigma = \frac{1}{L^{d-1}} Y(atL^{1/\nu}) \tag{1.5}$$

where, with the inclusion of the metric factor $a$, the function $Y(x)$, and thus $\Sigma(0)$, should be universal.[19] The choice of $a$ depends upon the convention adopted for $Y(x)$. If the choice $a = \sigma_0^{1/\mu}$ is made, then it follows that

$$Y(x) \sim x^{\nu(d-1)} \qquad \text{for} \quad x \to \infty \tag{1.6}$$

In this article $\Sigma$ and similar quantities are in units of $kT_c$.

For additional or more complete information on the critical phenomena at interfaces, the reader should consult refs. 20 and 21. The reviews in refs. 22 and 23 give a good introduction to the general theory of finite-size scaling, and have extensive references to the original literature. The two pieces of work with which this article is closely related,[2, 3] in addition to a collection of other articles dealing with finite-size scaling, can be found reprinted in ref. 24.

The organization of the article is as follows. Section 2 discusses the appropriate partition functions and expression for the surface tension. In Section 3 the mean field theory for such a system is considered. Section 4 concerns the effects of including low-order fluctuation corrections. In Section 5 the interfacial free energy is compared with some existing simulation data. Section 6 includes some discussion of the results and concluding remarks. Some further details are discussed in the Appendix.

## 2. PARTITION FUNCTIONS

Consider an Ising-like system contained in a hypercubic box of linear extent $L$ and volume $L^d$. As usual when considering critical behavior, the partition function may be written as

$$Z = \int \mathcal{D}\phi \, e^{-\mathcal{H}[\phi]} = e^{-\mathcal{F}} \tag{2.1}$$

where $\mathscr{H}[\phi]$ is a reduced Hamiltonian of the Landau–Ginzburg–Wilson form

$$\mathscr{H}[\phi] = \int d^d x \left[ \frac{1}{2} (\nabla\phi)^2 + \frac{r}{2}\phi^2 + \frac{u}{4!}\phi^4 \right] \tag{2.2}$$

In the sum over field configurations for the partition function, a set of boundary conditions is understood. For the present case of a planar interface, the free energies appropriate to a system of two coexisting phases and that of one uniform phase must be considered.

For the two-phase system, so as to address the free energy *intrinsic* to the interface, antiperiodic boundary conditions are imposed in one of the dimensions and periodic conditions in the remaining $d-1$ dimensions. These conditions effectively eliminate the boundary of the sample, and allow the center of the interface to sit anywhere in the longitudinal direction perpendicular to the interface. In the $d-1$ transverse directions parallel to the interface there is translational invariance. For the one-phase or uniform system, periodic conditions are imposed in all $d$ dimensions. If $\mathscr{F}_p$ and $\mathscr{F}_a$ denote the free energies for the one- and two-phase systems, respectively, then the interfacial free energy $\Sigma$ and surface tension $\sigma$ are defined by

$$\Sigma = \mathscr{F}_a - \mathscr{F}_p = \ln(Z_p/Z_a) \tag{2.3}$$

$$\sigma = \frac{\Sigma}{L^{d-1}} \tag{2.4}$$

In order for this definition to be meaningful, the configurations that effectively enter the partition sum should be those involving one interface. In the strong finite-size regime $tL^{1/\nu} \ll 1$, this criterion is certainly satisfied. On the other hand, for $tL^{1/\nu} \gg 1$, this criterion will be met so long as the aspect ratio, which is unity in this article, is not too large.

The evaluation of the partition functions $Z_{a,p}$ in a finite volume proceeds in very much the same way as that for a bulk system, except for two additional features. One of these is that certain modes will have to be treated nonperturbatively. The other is that the lattice sums, which normally go over into integrals, must be dealt with appropriately. Putting aside the treatment of the lattice sums for the moment, so as to clarify what is meant by the special treatment of modes, consider what is done for the uniform system. First, a shift in the field

$$\phi(\mathbf{x}) = m + \sigma(\mathbf{x}) \tag{2.5}$$

is made, where $m$ is constant, and is the entire $\mathbf{k}=\mathbf{0}$ part of $\phi(\mathbf{x})$. The variables are then changed to $\sigma_{\mathbf{k}}$, where

$$\sigma(\mathbf{x})=\frac{1}{L^{d/2}}\sum_{\mathbf{k}\neq\mathbf{0}}\sigma_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}} \tag{2.6}$$

with corresponding measure

$$\mathscr{D}\phi\to L^{d/2}\frac{dm}{\sqrt{2\pi}}\prod_{\mathbf{k}\neq\mathbf{0}}\frac{d\sigma_{\mathbf{k}}}{\sqrt{2\pi}}\equiv dm\,\mathscr{D}\sigma' \tag{2.7}$$

The uniform system partition function may thus be cast in the form

$$Z_{\mathrm{p}}=\int dm\,e^{-H_{\mathrm{p}}(m)}e^{-\Gamma_{\mathrm{p}}(m)} \tag{2.8}$$

where

$$H_{\mathrm{p}}(m)=L^{d}\left(\frac{rm^{2}}{2}+\frac{um^{4}}{4!}\right)=\mathscr{H}[m] \tag{2.9}$$

$$e^{-\Gamma_{\mathrm{p}}(m)}=\int\mathscr{D}\sigma'\,e^{-\Delta\mathscr{H}_{\mathrm{p}}[\sigma,m]} \tag{2.10}$$

$$\Delta\mathscr{H}_{\mathrm{p}}\equiv\int d^{d}x\left[\frac{1}{2}(\nabla\phi)^{2}+\left(r+\frac{um^{2}}{2}\right)\frac{\sigma^{2}}{2}+\frac{um\sigma^{3}}{3!}+\frac{u\sigma^{4}}{4!}\right] \tag{2.11}$$

The contribution to $\Gamma_{\mathrm{p}}(m)$ is expanded in the standard perturbative manner. In the above, and throughout the rest of the paper, the subscripts $\{\mathrm{p},\mathrm{a}\}$ refer to quantities for the one-phase and two-phase systems, respectively.

The above approach can be viewed as effectively introducing a moving saddle point, in that one sweeps over different values of $\langle\phi\rangle$ about which an expansion in fluctuations is performed. In the present circumstance, this is essential to maintaining the analyticity of the free energy. Quite often a saddle point expansion in a singular procedure that represents quantities normally well behaved in their arguments, as a sum, in many cases asymptotic, of nonanalytic terms. For example, consider the case at hand, which involves

$$Z_{\mathrm{p}}^{\mathrm{mf}}=\int dm\,e^{-H_{\mathrm{p}}(m)} \tag{2.12}$$

which is a well-behaved function of $r$ for *finite* $L$ and $u>0$. However, at leading order in a saddle point or large-$L$ expansion, the second derivative

with respect to $r$ of $\ln Z_p^{mf}$ is discontinuous. It is also instructive to note that if a usual saddle point expansion is attempted, then the lowest mode eigenvalue takes the form

$$\lambda_0 \sim |r| L^{1/\nu} \tag{2.13}$$

and thus becomes unstable for sufficiently small $r$. Inspection of $\mathscr{H}$, however, reveals that this limit should not be singular.

Consider now the two-phase system. As with the uniform system, if one attempts a straightforward loop expansion, the same type of problem encountered above occurs. In fact, the situation is worse in that the *two* lowest modes (in the ordered phase) are of the form

$$\lambda_0 = 0 \tag{2.14}$$

$$\lambda_1 \sim |r| L^{1/\nu} \tag{2.15}$$

Physically this might be expected since in the two-phase system the onset of order has the additional consequence of breaking translational invariance. These two modes, which in the bulk limit go over into the two bound states, are known in the literature as the translation and breathing modes. It is thus necessary to treat both these modes collectively. The treatment of the translation mode is accomplished by introducing a coordinate $z_0$ for the position of the interface center. As will become clear below, the treatment of the breathing mode is accomplished by integrating over profiles with different amplitude $m$, one of which is depicted in Fig. 1. This degree of freedom is the analog to that introduced in the one-phase system.

The sum over configurations in the two-phase partition function will be arranged into a sum over profiles and fluctuations about these profiles. Thus, consider a profile $\bar{\phi}(z)$, where $z$ is in the longitudinal direction. For

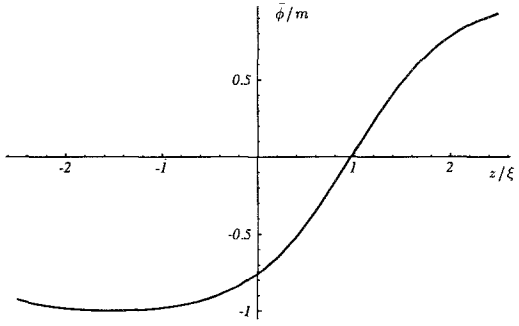


Fig. 1. A profile $\bar{\phi}$ corresponding to $L/\xi = 5$ and $z_0/\xi = 1$. In the limits $L/\xi \to \infty$ and $L/\xi \to \pi$ the curve becomes that of a translated $\tanh(x)$ and $\sin(x)$, respectively.

the moment assume that the profile center $\bar{\phi}=0$ is at $z=0$. The profile is chosen to satisfy

$$\bar{\phi}(L/2)=m=-\bar{\phi}(-L/2) \tag{2.16}$$

$$\left.\frac{d\bar{\phi}}{dz}\right|_{z=L/2}=0 \tag{2.17}$$

and the equation of state at some reduced temperature $r(m)$, that is,

$$-\frac{d^2\bar{\phi}}{dz^2}+r(m)\bar{\phi}+\frac{u\bar{\phi}^3}{3!}=0 \tag{2.18}$$

where $r(m)$ is chosen so that $\bar{\phi}$ has one zero crossing. By now considering the extension of this function to $|z|>L/2$, it follows that $\bar{\phi}(z-z_0)$ is a solution to the equation of state 2.18 and satisfies the antiperiodic boundary condition. The function $\bar{\phi}$, which depends on $m$ in addition to $z$, will be discussed in greater detail below.

The collective treatment of the variables $m$, $z_0$ presented here is patterned after that of Gervais and Sakita.[25] Begin by considering the two functions

$$y_1(z_0, m)=\int d^dx\,\bar{\phi}(z-z_0, m)[\phi-\bar{\phi}] \tag{2.19}$$

$$y_2(z_0, m)=\int d^dx\,\frac{\partial\bar{\phi}}{\partial z_0}(z-z_0, m)[\phi-\bar{\phi}] \tag{2.20}$$

along with the identity

$$\int d^2y\,\delta(\mathbf{y})=1 \tag{2.21}$$

Now *assume* that the above transformation is well defined enough so that one can write

$$1=\int d^2y\,\delta(\mathbf{y})=\int dz_0\,dm\,J(z_0, m)\,\delta[\mathbf{y}(z_0, m)] \tag{2.22}$$

where the Jacobian $J$ is given by

$$J=\left|\det\left(\frac{\partial y_i}{\partial u_j}\right)\right| \tag{2.23}$$

with

$$u_1=z_0, \qquad u_2=m \tag{2.24}$$

These coordinates are then introduced into the partition function by inserting the decomposition of unity (2.22) into $Z$, from which it follows that

$$Z_a = \int dz_0\, dm\, J[\sigma, m, z_0] \exp(-\mathscr{H}[\bar{\phi}] - \Delta\mathscr{H}_a)\, \delta[\mathbf{y}]$$

$$\equiv \int dz_0\, dm \exp[-H_a(m, z_0) - \Gamma_a(m, z_0)] \tag{2.25}$$

where

$$H_a(m, z_0) = \mathscr{H}[\bar{\phi}] = \int d^d x \left[\frac{(\nabla\bar{\phi})^2}{2} + \frac{r\bar{\phi}^2}{2} + \frac{u\bar{\phi}^4}{4!}\right] \tag{2.26}$$

$$\Delta\mathscr{H}_a = \int d^d x \left[\frac{(\nabla\sigma)^2}{2} + \left(r + \frac{u\bar{\phi}^2}{2}\right)\frac{\sigma^2}{2} + \frac{u\bar{\phi}}{3!}\sigma^3 + \frac{u}{4!}\sigma^4\right] \tag{2.27}$$

$$e^{-\Gamma_a} = \int \mathscr{D}\sigma\, J e^{-\Delta\mathscr{H}_a} \delta(\mathbf{y}) \tag{2.28}$$

Effectively, $\int d^d x\, \sigma\bar{\phi} = 0$ in $\Delta\mathscr{H}$ because of the $\delta$ function and the choice of $y_1$.

The choice of the functions $y_i$ is to some extent arbitrary, and dictated by convenience. The Jacobian will ensure that the partition function will remain invariant independent of the specific choice of transformation functions adopted. By now the use of the function $y_2$ for the translation mode is standard. This constraint effectively clamps the interface so that a stable integration over the fluctuations $\sigma$ may be effected. The contribution associated with a collective translation of the interface yields an entropic factor of $L$ through the integration over $z_0$. A detailed account of the rationale that leads to the choice of the function $y_1$ can be found in ref. 29. Here it will only be mentioned that the above choice is motivated by the coincidence of $\bar{\phi}$ with the breathing mode in the strong finite-size regime and the desire to obtain a simple form of interaction $\Delta\mathscr{H}$.

## 3. MEAN FIELD THEORY

Consider the approximation of ignoring the effects of fluctuations about the configurations $\bar{\phi}$. This is achieved by setting $\phi = \bar{\phi}_{a,p}$ and tracing over $\bar{\phi}_{a,p}$ in both the partition functions. In the thermodynamic limit this level of approximation will retain terms of order $1/u$ to the free energy. For a finite system, however, the integration over $m$ will have the effect of

mixing different orders in perturbation theory. In particular, such an integration leads naturally to retaining terms of order unity in the coupling. It also gives rise to an interfacial free energy with a logarithmic dependence on $u$ at the bulk critical point. This dependence in itself generally would require one to consider terms of order unity in $u$. As the loop correction is also order unity, a consistent account of such terms leads to consideration of the loop term. Hence, in the present circumstance, a mean field approximation based on neglecting the loop correction is problematic. The results of this section are thus qualitative, and presented primarily for purposes of illustration.

With the above in mind, setting $\exp(-\Gamma_{a,p}) = 1 = J$, it follows that in this approximation,

$$Z_p = \int dm \exp(-\mathscr{H}[\bar{\phi}_p]) = \int dm \exp\left[-L^d\left(\frac{rm^2}{2} + \frac{um^4}{4!}\right)\right] \tag{3.1}$$

$$Z_a = \int dm \exp(-\mathscr{H}[\bar{\phi}_a]) = \int dm \exp[-H_a(m)] \tag{3.2}$$

This essentially corresponds to an expression that would be written down if one paid *no* attention to fluctuation corrections other than the need to integrate over $m$, which follows naturally from Landau theory.

In order to proceed, it is necessary to determine the function $H_a(m)$. To this end, first note that the profile satisfying the equation of state (2.18) is given by

$$\bar{\phi}_a(z) = m \operatorname{sn}\left(\frac{z}{\xi}\right) \tag{3.3}$$

where $\operatorname{sn}(x)$ is one of the standard Jacobian elliptic functions (see, e.g., ref. 35). The coordinate $z_0$ has been set to zero, as the integration over $z_0$ gives only an additional multiplicative factor. The modulus $k$ of the elliptic function, the correlation length $\xi$, and the reduced temperature $r(m)$ are given by

$$kK(k) = \left(\frac{uL^2m^2}{48}\right)^{1/2} \tag{3.4}$$

$$\xi = \frac{L}{2K} \tag{3.5}$$

$$r(m) = -\frac{um^2}{12}\left(\frac{1}{k^2} + 1\right) \tag{3.6}$$

where $K(k)$ is the complete elliptic integral of the first kind (see, e.g., ref. 35). For $r \geqslant -(\pi/L)^2$ there is no profile, that is, $\bar{\phi}_a = 0$ is the solution to the equation of state (2.18). This is in accord with the expectation that a nominal transition temperature should shift by $\delta r \sim 1/L^{1/\nu}$. The function $H_a(m)$ is obtained by substituting $\bar{\phi}_a$ into $\mathscr{H}[\phi]$. The result is

$$H_a = \frac{24K}{uL^{\varepsilon}} \left\{ (K-E) \left[ rL^2 + \frac{4K^2}{3}(1+k^2) \right] + \frac{4}{3} k^2 K^3 \right\} \tag{3.7}$$

where $E(k)$ is the complete elliptic integral of the second kind.

In Fig. 2 the surface tension $\sigma$ in four dimensions is plotted for several values of the linear system size $L$. It is clear that $\sigma$ is smooth across $r = 0$ (or actually the shifted temperature) when the behavior of the curve is considered on a scale $\Delta r < 1/L^2$. This behavior is completely analogous to that found in ref. 2. However, the overall smooth nature of the curves in Fig. 2 is to some extent dependent on the inclusion of terms formally of higher order than $1/u$. Though not apparent from the figure, it happens that for sufficiently high temperatures the surface tension becomes negative. This disaster results from both the incorrect normalization of the measure and inclusion of terms of higher order in the coupling than those consistently accounted for. To obtain the proper behavior in this regime it is necessary both to work at least to one-loop order and to reassess the present approach. In particular, a consistent approach will ultimately have to abandon the hope of obtaining *globally* smooth curves for the interfacial tension.

In the present circumstance $\Sigma(0)$ is not expected to be universal, or for that matter, independent of $L$. Inspection of the curves, however, indicates

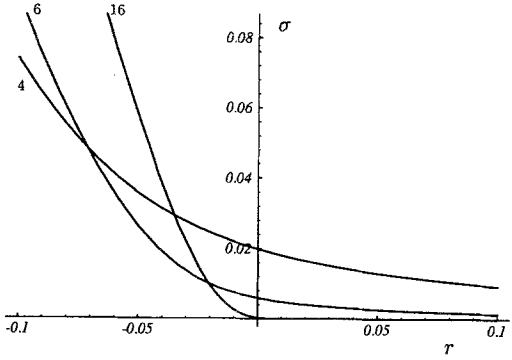


Fig. 2. The surface tension $\sigma$ in mean field approximation for various values of $L$ with coupling $u = 1$.

that $\Sigma(0)$ depends very weakly on $L$. Due to the manner in which the Jacobians and loop terms were dealt with, this is entirely accidental. This behavior may be understood by noting that because of the depressed transition temperature of the two-phase system, at $r=0$ only profiles with small moduli should effectively enter. It is then reasonable to approximate $H_a$ by the first term of an expansion in the modulus $k$,

$$H_a \simeq \frac{L^d}{4}\left(\frac{\pi m}{L}\right)^2 \tag{3.8}$$

This approximation becomes better as $u$ becomes smaller. Upon a change of variable $s=Lm$ in $Z_{a,p}$, the $L$ dependence cancels and

$$\frac{Z_p}{Z_a} \simeq \frac{\int_{-\infty}^{\infty} ds \exp[-(u/4!)s^4]}{\int_{-\infty}^{\infty} ds \exp[-(\pi s)^2/4]} \tag{3.9}$$

which gives

$$\Sigma(0) \simeq \frac{1}{4}\ln\left[\frac{24\pi^2\Gamma(5/4)^4}{u}\right] \tag{3.10}$$

This expression agrees within a couple percent with that of the curves for values of $u<10$, with better agreement for smaller $u$. The above illustrates one manner in which terms of $\ln(u)$ may enter the free energy. It also happens that the Jacobian gives rise to such terms below the critical point.

## 4. FLUCTUATION CORRECTIONS

This section addresses the manner in which leading fluctuations are included in the free energy. In order to treat these fluctuations in a convergent manner, it is necessary to implement the renormalization group. This amounts to successively integrating out all high-momentum modes until the block size $e^l \simeq \min(L, \xi)$, at which point a loop expansion may then be performed.[26] This is done for the uniform system following refs. 2 and 26. For the nonuniform system, a similar approach is taken,[8] of which a brief account follows. A shift in the field is made,

$$\phi = \bar{\phi} + \sigma \tag{4.1}$$

and the parameters $r(l)$, $u(l)$ are taken to flow according to the disordered phase recursion relations

$$\frac{dr}{dl} = 2r + \left(\frac{K_d}{2}\right)\frac{u}{1+r} \tag{4.2}$$

$$\frac{du}{dl} = \varepsilon u - \left(\frac{3K_d}{2}\right)\frac{u^2}{(1+r)^2} \tag{4.3}$$

while the average of the field flows as

$$\bar{\phi}(\mathbf{x}, l) = e^{(d-2+\eta)l/2}\bar{\phi}(\mathbf{x}e^{l}, 0) \tag{4.4}$$

The recursion relations are stopped when

$$t(l^*) + \frac{g(l^*)}{2}\langle\bar{\phi}(l^*)^2\rangle + \frac{1}{L(l^*)^2} = 1 \tag{4.5}$$

where $t(l)$, $g(l)$, $L(l)$ are given by

$$t(l) = r(l) + \frac{K_d u(l)}{4} - \frac{K_d r(l)\, u(l)}{4}\ln[1 + r(l)] \tag{4.6}$$

$$g(l) = u(l) - \frac{3}{4}K_d u(l)^2\left\{\ln[1 + r(l)] + \frac{r(l)}{1 + r(l)}\right\} \tag{4.7}$$

$$L(l) = e^{-l}L \tag{4.8}$$

and the phase space factor $K_d = [2^{d-1}\pi^{d/2}\Gamma(d/2)]^{-1}$. The average $\langle\bar{\phi}^2\rangle$ appearing in (4.5) is discussed below. An approximate integration of the RG equations (4.2), (4.3) reveals that[26] these parameters evolve according to

$$g(l) = \frac{ue^{\varepsilon l}}{Q(l)} \tag{4.9}$$

$$t(l) = \frac{t(0)e^{2l}}{Q(l)^{1/3}} \tag{4.10}$$

where

$$Q(l) = 1 + (u/u^*)(e^{\varepsilon l} - 1) \tag{4.11}$$

Upon integrating out the field $\sigma$, it is possible to show that when account is taken of the trajectory integral, bare quantities may effectively be replaced by renormalized ones, along with appending appropriate bulk subtractions.

From this point on, all parameters refer to renormalized ones (their value at $l^*$), and the following notation is adopted:

$$(\psi, \phi) = \int d^d x\, \psi\phi \tag{4.12}$$

$$(\psi, G\phi) = \int d^d x\, d^d x'\, \psi(\mathbf{x})\, G(\mathbf{x}, \mathbf{x}')\, \phi(\mathbf{x}') \tag{4.13}$$

$$\|\psi\| = (\psi, \psi)^{1/2} \tag{4.14}$$

Consider now the contributions to $\Gamma(m^2)$ arising from the Gaussian fluctuations. For the one-phase system these follow immediately from

$$\int \mathscr{D}\sigma' \, e^{-(\sigma, G_p^{-1}\sigma)/2} = \frac{L^{d/2}}{(2\pi)^{1/2}} \frac{1}{(\det' G_p^{-1})^{1/2}} \tag{4.15}$$

where the prime denotes omission of the lowest ($\mathbf{k}=\mathbf{0}$) eigenvalue. Similarly, for the two-phase system it is straightforward to show that

$$\int \mathscr{D}\sigma \, J e^{-(\sigma, G_a^{-1}\sigma)/2} \delta(\mathbf{y}[\sigma]) = \frac{(\bar{\phi}_a, \partial\bar{\phi}_a/\partial m)}{2\pi(\det' G_a^{-1})^{1/2}} \left[\frac{(\partial\bar{\phi}_a/\partial z, \partial\bar{\phi}_a/\partial z)}{(\bar{\phi}_a, G_a'\bar{\phi}_a)}\right]^{1/2}$$

$$\equiv \frac{\mathscr{J}}{(\det' G_a^{-1})^{1/2}} \tag{4.16}$$

Some comments regarding this latter result now follow. In obtaining this result, the $\sigma$ dependence of $J$ has been ignored, so that

$$J \simeq \left(\frac{\partial\bar{\phi}_a}{\partial z_0}, \frac{\partial\bar{\phi}_a}{\partial z_0}\right)\left(\bar{\phi}_a, \frac{\partial\bar{\phi}_a}{\partial m}\right) \tag{4.17}$$

The prime on the determinant omits the lowest (translation mode) eigenvalue of the operator $G_a^{-1}$ which is given by

$$G_a^{-1}(\mathbf{x}, \mathbf{x}') = \left(-\nabla^2 + t + \frac{g\bar{\phi}_a^2}{2}\right)\delta^d(\mathbf{x}-\mathbf{x}') \tag{4.18}$$

where to order $u$ the replacement $r \to t$, $u \to g$ has been made. Similarly, $G'$ is the projected propagator

$$G_a'(\mathbf{x}, \mathbf{x}') = G_a(\mathbf{x}, \mathbf{x}') - \frac{\psi_0(z)\,\psi_0(z')}{\lambda_0} \tag{4.19}$$

which may be replaced by $G_a$ since $\bar{\phi}_a$ has no overlap with $\psi_0$. The factor $\mathscr{J}$ may be written in the form

$$\mathscr{J} = \frac{1}{2\pi\langle G_a\rangle^{1/2}} \left\| \frac{\partial\bar{\phi}_a}{\partial z} \right\| \frac{\partial \, \|\bar{\phi}_a\|}{\partial m} \tag{4.20}$$

where

$$\langle G_a\rangle \equiv \frac{(\bar{\phi}_a, G_a\bar{\phi}_a)}{(\bar{\phi}_a, \bar{\phi}_a)} \tag{4.21}$$

In the expression for $\mathscr{J}$, the factor $\langle G_a \rangle$ may be interpreted as arising because $\bar{\phi}_a$ is *not* an eigenmode of the fluctuation operator. This factor tends to cancel terms from the determinant that have already been accounted for by the integration over profiles.

Before proceeding with the explicit evaluation of these formulas, an important mode of approximation is discussed. As both partition functions are of the form

$$Z = \int dm\, e^{-H(m^2)} e^{-\Gamma(m^2)} \tag{4.22}$$

it appears that the function $\Gamma(m^2)$ must be evaluated for general $m$. Such a global evaluation of $\Gamma$ is, however, both problematic and unnecessary. Allowing $m^2$ to vary over all positive values will in principle cause additional modes to become unstable. This problem is circumvented by exploiting the perturbative nature of the calculation to organize an expansion about a suitable value of $m^2$. It can be shown[29] that to order $u^0$ the replacement

$$\Gamma(m^2) \to \Gamma(\langle m^2 \rangle) \tag{4.23}$$

may be made, where the average $\langle m^2 \rangle$ is computed with the weight $\exp[-H(m^2)]$. While this is strictly true for the one-phase system, additional care must be exercised with the two-phase system, since $\mathscr{J}$ takes the form

$$\mathscr{J} = |m|\, e^{y(gm^2)} \equiv m j(m^2) \tag{4.24}$$

with $y(0)$ nonsingular. This naturally leads to the weight $|m| \exp(-H_a)$ for the two-phase system. Thus, the explicit forms adopted for the averages are

$$\langle m^2 \rangle_p = \frac{\int dm\, m^2 e^{-H_p}}{\int dm\, e^{-H_p}}, \qquad \langle m^2 \rangle_a = \frac{\int dm\, |m|^3\, e^{-H_a}}{\int dm\, |m|\, e^{-H_a}} \tag{4.25}$$

Finally, analysis of the loop correction reveals that part of this term has the effect of replacing the parameters $r$, $u$ in $H$ by their shifted counterparts $t$, $g$.

Returning now to the explicit evaluation of the fluctuation corrections, the two Fredholm determinants appearing in (4.15), (4.16) make a contribution of

$$\frac{1}{2} \ln \left[ \frac{\det(-\nabla^2 + t + \frac{1}{2} g \langle \bar{\phi}_a^2 \rangle)_a}{\det(-\nabla^2 + t + \frac{1}{2} g \langle \bar{\phi}_p^2 \rangle)_p} \right] \equiv \frac{1}{2} \ln D \tag{4.26}$$

to the interfacial free energy. The order of the calculation permits the replacement of $r$, $u$ by $t$, $g$ in this expression. The averages $\langle \bar{\phi}^2_{\mathrm{p,a}} \rangle$ correspond to those mentioned above, namely for the uniform system

$$\langle \bar{\phi}^2_{\mathrm{p}} \rangle \equiv \langle m^2 \rangle_{\mathrm{p}} \tag{4.27}$$

while for the two-phase system

$$\langle \bar{\phi}^2_{\mathrm{a}} \rangle \equiv \bar{\phi}^2(z; \langle m^2 \rangle_{\mathrm{a}}) \tag{4.28}$$

The subscripts a and p on the determinants refer to the boundary conditions imposed in the direction perpendicular to the interface. The periodic conditions in the remaining $d-1$ dimensions imply that

$$\ln D = \sum_{\mathbf{q}} \ln \left[ \frac{\det(-\partial_z^2 + q^2 + t + \frac{1}{2} g \langle \bar{\phi}^2_{\mathrm{a}} \rangle)_{\mathrm{a}}}{\det(-\partial_z^2 + q^2 + t + \frac{1}{2} g \langle \bar{\phi}^2_{\mathrm{p}} \rangle)_{\mathrm{p}}} \right] \tag{4.29}$$

where the variable $\mathbf{q}$ is a $(d-1)$-dimensional vector with components

$$q_\alpha = \frac{2\pi}{L} n_\alpha, \qquad n_\alpha = 0, \pm 1, \pm 2, \ldots \tag{4.30}$$

Using the short-hand notation

$$\ln D = \sum_{\mathbf{q}} \ln \left[ \frac{\det(A_{\mathrm{a}} + q^2)}{\det(A_{\mathrm{p}} + q^2)} \right] \equiv \sum_{\mathbf{q}} \ln[d(q^2)] \tag{4.31}$$

it follows that

$$\ln D = \int_0^\infty \frac{ds}{s} \left( \sum_{\mathbf{q}} e^{-sq^2} \right) [\mathrm{Tr}\, e^{-sA_{\mathrm{p}}} - \mathrm{Tr}\, e^{-sA_{\mathrm{a}}}] \equiv \int_0^\infty ds\, F(s) \tag{4.32}$$

This integral is broken up into two parts,

$$\int_0^\infty F(s) = \int_0^B ds\, F(s) + \int_B^\infty ds\, F(s) \tag{4.33}$$

where the constant $B$ is chosen to be of order $L^2$. The natural choice $B = 4\pi L^2$ allows good convergence and is ultimately made. In the first term the Poisson summation formula

$$\sum_{\mathbf{q}} f(\mathbf{q}) = \left( \frac{L}{2\pi} \right)^{d-1} \sum_{\mathbf{m}} \int d^{d-1} q\, e^{iL\mathbf{q}\cdot\mathbf{m}} f(\mathbf{q}) \tag{4.34}$$

is used. By noting that the $\mathbf{m}=\mathbf{0}$ term is the bulk contribution, it follows after some changes of variables that

$$\ln D' = \left(\frac{L}{2\pi}\right)^{d-1} \int d^{d-1}q \ln[d(q^2)]$$
$$+ \int_1^\infty ds\, s^{(d-3)/2}[\Theta^{d-1}(\pi s) - 1]\, T\left(\frac{L^2}{4\pi s}\right)$$
$$+ \int_1^\infty \frac{ds}{s}[\Theta^{d-1}(\pi s) - (1/s)^{(d-1)/2}]\, T\left(\frac{L^2 s}{4\pi}\right) - \ln\left(\frac{\lambda^{\mathrm{a}}}{\lambda^{\mathrm{p}}}\right) \quad (4.35)$$
$$\equiv \left(\frac{L}{2\pi}\right)^{d-1} \int d^{d-1}q \ln[d(q^2)] + 2\Sigma^{\mathrm{fs}} \quad (4.36)$$

The functions $T$ and $\Theta$ are defined by

$$T(x) = \mathrm{Tr}\, e^{-xA_{\mathrm{p}}} - \mathrm{Tr}\, e^{-xA_{\mathrm{a}}} \quad (4.37)$$

$$\Theta(x) = \sum_{-\infty}^{\infty} e^{-xn^2} \quad (4.38)$$

and $\lambda^{\mathrm{p,a}}$ are the lowest eigenvalues of the operators $A_{\mathrm{p,a}}$.

This expression for the finite-size correction is not yet in a usable form. The two lowest eigenvalues, while always positive for a finite system, may vanish with $L$ more rapidly than $1/L^2$. The integral over the trace (4.35) may thus become divergent. This divergence, however, will be canceled by the eigenvalues that have been subtracted off. By separating these two modes out of the trace in the third term above, a convergent expression that involves the exponential integral and error function is found. As this expression is somewhat formidable, it is recorded elsewhere.[29] For the evaluation of the traces and function $\Theta$ it is sufficient to keep only the first several terms.

It was previously noted that the lowest eigenvalue of $A_{\mathrm{a}}$, the translation mode, was *positive* rather than identically zero. The reason for this is that profiles enter the partition sum that do not extremize $\mathscr{H}$. The degree to which this happens is determined by a well $L^d$ deep which governs fluctuations of the magnetization of each domain bounding the interface. As a consequence, this "zero mode" will be null only to the extent that the configurations effectively entering tend to be coincident with the minimum of this well. It thus follows that

$$\lambda^{\mathrm{a}} \sim \frac{1}{L^d} \quad (4.39)$$

Because $\lambda^a$ may become small and the saddle point $\bar{\phi}$ is degenerate in $z_0$, this mode, while not strictly vanishing, must still be treated collectively.

Consider now the evaluation of the Fredholm determinant $d(q^2)$. It can be shown that[29]

$$\frac{\det[-\partial_z^2+(u/2)\langle\bar{\phi}_a^2\rangle-\lambda]_a}{\det[-\partial_z^2+(u/2)\langle\bar{\phi}_p^2\rangle-\lambda]_p}=-\frac{\sinh^2(\rho K)}{\sinh^2(\frac{1}{2}L\sqrt{\kappa})} \tag{4.40}$$

where $K$ is the same as that of (3.4) and[36]

$$\rho=\frac{\operatorname{sn}\omega\operatorname{cn}\omega\operatorname{dn}\omega}{\operatorname{sn}^2 a-\operatorname{sn}^2\omega}-Z(\omega) \tag{4.41}$$

$$\kappa=\frac{u}{2}\langle\bar{\phi}_p^2\rangle-\lambda \tag{4.42}$$

with

$$\operatorname{sn}^2\omega=\frac{\operatorname{sn}^4 a\,(2k^2\operatorname{sn}^2 a-1-k^2)}{3k^2\operatorname{sn}^4 a-2(1+k^2)\operatorname{sn}^2 a+1} \tag{4.43}$$

$$\operatorname{sn}^2 a=\frac{4(1+k^2)-\lambda\xi^2}{6k^2} \tag{4.44}$$

Here $\xi$ is that of (3.5), $k$ the modulus of the elliptic function (3.4), and $Z$ the Jacobi zeta function (see, e.g., ref. 35). The Appendix briefly discusses some properties of the fluctuation operator $[A_a-\lambda]$; further details can be found in ref. 29.

By combining the above results, it is now possible to determine the interfacial free energy $\Sigma$,

$$\Sigma=\Sigma^{\mathrm{rmf}}+\Sigma^{\mathrm{lp}}+\Sigma^{\mathrm{fs}} \tag{4.45}$$

These three terms are respectively the contributions from renormalized mean field theory, the loop term, and the finite-size correction. The renormalized mean field (rmf) level of approximation replaces bare parameters in the mean field approximation by shifted and renormalized ones,

$$\Sigma^{\mathrm{rmf}}=\ln(Z_p^{\mathrm{rmf}}/Z_a^{\mathrm{rmf}}) \tag{4.46}$$

$$Z_p^{\mathrm{rmf}}=\int dm\, e^{-H_p} \tag{4.47}$$

$$Z_a^{\mathrm{rmf}}=\int |m|\, dm\, e^{-H_a} \tag{4.48}$$

This is accomplished by including that part of the trajectory integral which contributes to the mass and interaction terms. This level of approximation gives the order-$\varepsilon$ corrections to the classical exponents, and in four dimensions yields results correct to leading logarithms. The loop contribution, which also includes the contribution from the Jacobian(s), is defined by

$$\Sigma^{\text{lp}} = \frac{1}{2}\left(\frac{L}{2\pi}\right)^{d-1} \int d^{d-1}q \ln[d(q^2)] - S + \ln\left(\frac{L^{d/2}}{Lj\sqrt{2\pi}}\right) \tag{4.49}$$

where the subtraction is given by

$$S = \frac{g}{4}\int d^d x \,(\langle \bar{\phi}_{\text{a}}^2 \rangle - \langle \bar{\phi}_{\text{p}}^2 \rangle)\left[\int \frac{d^{d-1}q}{(2\pi)^{d-1}} \frac{\theta(q-1)}{2(q^2+t)^{1/2}} + f(t)\right]$$
$$-\left(\frac{g}{4}\right)^2 \int d^d x \,(\langle \bar{\phi}_{\text{a}}^2 \rangle^2 - \langle \bar{\phi}_{\text{p}}^2 \rangle^2)\left[\int \frac{d^{d-1}q}{(2\pi)^{d-1}} \frac{\theta(q-1)}{4(q^2+t)^{3/2}} - \frac{\partial f}{\partial t}\right] \tag{4.50}$$

with

$$f(t) = K_4\{(1+t)^{1/2} - t\ln[1+(1+t)^{1/2}]\} \tag{4.51}$$

This term is arrived upon by integrating out $k_z$ from the usual hard cutoff subtraction. Part of the contributions to $f$ and $f'$ have been used to replace $r$, $u$ by $t$, $g$ in the functions $H_{\text{a}}$, $H_{\text{p}}$ appearing in (4.47), (4.48). The extra factor of $L$ in (4.49) comes from the integration over the coordinate $z_0$. Finally, the contribution arising from the finite-size corrections to the lattice sum is given by (4.36).

## 5. NUMERICAL RESULTS

Before attempting to make comparisons with the simulations, it is necessary to consider in more detail the actual calculation of the scaling function. As it stands, the calculation requires an "exact" integration over a coordinate $m$ for both the one- and two-phase systems. If this is done, the scaling function that results consists of a single smooth curve that interpolates throughout the *entire* scaling regime. While this is an appealing feature, the resulting curve is both in very poor agreement with the simulations and qualitatively incorrect.[29] This comes as little surprise after it is realized that such an integration does not properly truncate terms at an order consistent with that of the entire calculation. Furthermore, there are also problems associated with setting epsilon to a finite number *prior* to computing the scaling function via a computer. What must be done is to extract those aspects of the nonperturbative treatment that are essential

to the calculation while simultaneously eliminating the higher-order terms. This program is possible if separate pieces of the scaling function are considered and the requirement that the pieces join smoothly together is relaxed. The primary reason for the occurrence of discontinuities is that the terms to be eliminated differ depending on whether the system is near, somewhat below, or somewhat above the critical point. While the discontinuities between the pieces are of order of the eliminated higher-order terms, they are nevertheless *finite* when the coupling takes on a noninfinitesimal value. In four dimensions the situation improves, provided the original coupling is small and the system size is large enough to permit partial crossover to the Gaussian fixed point.

## 5.1. Below Four Dimensions

In order to compare the interfacial tension of this article with that of a simulation, appropriate measures must be taken to account for the differing nonuniversal amplitudes. This is accomplished by invoking the assumption that *all* the nonuniversality is contained in the metric factor. It is thus possible to compare the functions $Y$ of Eq. (1.5), or equivalently the free energies, once the argument of one is suitably scaled. The correspondence between the two is

$$\Sigma^{(1)}(t) = \Sigma^{(2)}(bt) \tag{5.1}$$

where

$$b = \left(\frac{\sigma_0^{(1)}}{\sigma_0^{(2)}}\right)^{1/\mu} \tag{5.2}$$

and $\sigma_0^{(i)}$ are the amplitudes of the surface tension (1.1) for the respective systems.

Perhaps the most general aspect of the results is their scaling. An analysis of the free energy reveals that $\Sigma$ scales with argument $tL^{1/\nu}$. Though this might be expected, the literature is not particularly clear on this point. Presumably, because the system contains a "soft" mode, it is possible for nonscaling terms of the form $\ln L$ to enter the free energy.[16, 22] In the present analysis, however, it is found that the length always enters in the form of the scaling variable mentioned above. This is a consequence of the RG, which gives rise to the *renormalized* length $L^*$ (4.8) entering the expansion. The results of the simulations also support the scaling of the data. While it might be argued that the breakdown of scaling due to a $\ln L$ term is a small effect, the analysis of Mon[4] focuses primarily on these terms, and appears to indicate that the scaling variable enters the logarithm.

Turning now to the explicit results, the first "piece" of the scaling function considered is that appropriate to large negative $X$. It can be shown that,[29] to order $\varepsilon^0$,

$$\Sigma(t, L) = (\sigma_0^{1/\mu} |X|)^{\mu} - \frac{\mu}{2} \ln(\sigma_0^{1/\mu} |X|) + C + O(e^{-X^{\nu}/\sqrt{2}}) \tag{5.3}$$

where

$$X \equiv tL^{1/\nu} \tag{5.4}$$

$$\sigma_0 = \frac{4\sqrt{2}}{g^*}\left[1 + \frac{3K_d g^*}{8}\left(1 - \ln 2 - \frac{\pi}{3\sqrt{3}}\right)\right] \tag{5.5}$$

$$C = \frac{1}{2}\left(\gamma - \ln 2 + \frac{2}{3} - 0.167\right) \tag{5.6}$$

In deriving this result and those that follow, a contribution of $\ln g$ is regarded to be of slightly lower order than $g^0$, but of higher order than $1/g$. The limit of large $X$ is understood as $L \gg \xi$ while maintaining $\xi \gg 1$. The value of $\sigma_0$ follows from a bulk calculation using the conventions of this article, and is identical to that found in ref. 10, where dimensional regularization was used. The logarithmic factor in (5.3) includes, among other factors of $L$, those found in a drumhead analysis, and follows immediately from consideration of $\mathscr{J}$ and the finite-size term $\Sigma^{\text{fs}}$. The coefficient proceeding the logarithm is equivalent that already found in refs. 3 and 32. The leading exponential corrections appearing in (5.3) arise from the modulus $k$ differing from unity.

The data of the simulation[4] were fitted to a form

$$Y(X) \simeq |X|^{\mu} - A\mu \ln |X| \tag{5.7}$$

with

$$A = 0.66 \pm 0.12 \tag{5.8}$$

Inspection of Fig. 3 indicates that while 0.5 is just outside the quoted experimental error, if data for *large* $X$ are considered, a factor of 0.5 is not ruled out. It is possible that the exponential corrections in (5.3) may account for the bending of the data away from the line in Fig. 3. As the slope of the theoretical line is less than that found by Mon, it leads to an extrapolated value of $\sigma_0$ roughly 3% less than Mon's estimate. This accounts for some of the discrepancy between the value found by Mon and that of Meyer-Ortmanns and Trappenberg.[27] The latter authors extract the surface tension from a vacuum tunneling energy and obtain $\sigma_0 = 1.51$, which is 5% less than the estimate of Mon.

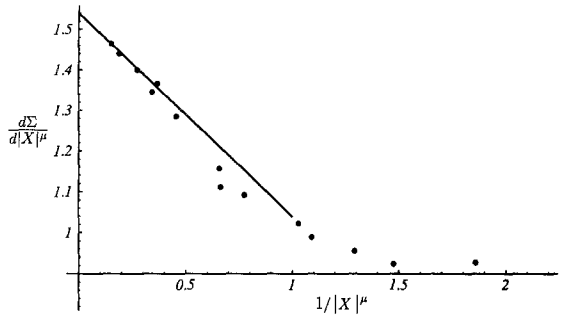


Fig. 3. Comparison between the simulation data of ref. 4 and the large-$|X|$ behavior given by (5.3). The intercept $\sigma_0 = 1.54$ has been adjusted to match the large-$|X|$ data with the line of fixed slope 0.5.

Estimates of factors *related* to $A$ have already appeared in the literature. The value of $A$ corresponding to a constrained drumhead model[28] which *excludes* the zero mode is $-1/(d-1)$. This value is entirely due to the capillary mode fluctuations, and differs from that of this article primarily because it does not include effects arising from a collective translation of the drumhead. Another result $(d-3)/(2d-2)$, found from a relation involving the surface tension and correlation length in a slab geometry, is reported in refs. 3 and 32. In two dimensions it agrees with the logarithmic factors found in exact calculations via a transfer matrix spectral gap. It is consistent with the result of this article after account is taken of an entropic factor of $L$ which has been factored away.[29]

The next piece of the scaling function considered is that appropriate to behavior very close to the bulk critical point, $X \ll 1$. In this regime $\Sigma$ is expected to be a linear function of $X$ with

$$\Sigma'(0) = \sigma^{1/\mu} Y'(0) \tag{5.9}$$

where $Y'(0)$ is universal. Assuming $X \sim \varepsilon$ and expanding about the quartic term in $H_p$, while keeping only the quadratic part of $H_a$, the result, which formally keeps terms to $\sqrt{\varepsilon}$, is[29]

$$\Sigma \simeq \frac{1}{4} \ln\left[\frac{2^9 3 \Gamma^4(5/4)}{g^*}\right] - \frac{\sqrt{24}\,\Gamma(7/4)}{6\Gamma(5/4)} \frac{X}{\sqrt{g^*}} + \frac{\pi^2}{48} - 0.74 - \frac{\sqrt{2g^*}\,\Gamma(7/4)}{16\pi\sqrt{3}\,\Gamma(5/4)}\left(\frac{\pi}{3} - 2.63\right) \tag{5.10}$$

where $\Gamma$ is the standard gamma function. Upon performing the above calculation, it happens that to the order considered, $\Sigma(0)$ is independent of

$L^*$. This is expected, as it implies the amplitude is independent of $l^*$. Furthermore, it is possible to show that both the entire expression of (5.10) along with those pertaining to the other two regimes (5.3), (5.15) are independent of $l^*$. The expression (5.10) indicates the manner in which the dangerous irrelevant variable $g$ enters the amplitude.

It is now possible to estimate both the value and slope of $\Sigma$ at the critical point; from (5.10) it follows that

$$Y(0) \simeq 0.64 \tag{5.11}$$

$$Y'(0) \simeq -0.51 \tag{5.12}$$

where use was made that $K_d g^* = 2\varepsilon/3$ and $\sigma_0 = 4\sqrt{2}/g^*$, which are appropriate to the order considered in this regime. Notice that unlike the first three terms in (5.3), the metric factor in (5.10) does not "naturally" appear in the argument of $Y$. The simulation results of ref. 5 give for the amplitude

$$Y(0) = 0.6 \pm 0.02 \tag{5.13}$$

Regarding the comments made at the beginning of this section, the result which follows from the exact integration over $m$ differs from the simulation value by a factor of five.

Concerning the value of the slope, the data of ref. 5 are somewhat peculiar in this respect. When the interfacial free energy is plotted against $X^\mu$, it is found that the data are rather well fitted by a line. This was naturally interpreted by the authors as having reached the large-$X$ asymptotic regime, even though the data were for somewhat small $X$. What seems odd is that when the line is extrapolated to $X = 0$, the intercept appears to coincide *exactly* with $\Sigma(0)$. This in principle cannot happen since $\Sigma$ is *linear* in $X$ for small argument. A plot versus $X^\mu$ is thus expected to have a small cusp accompanied perhaps by some bending, as was found in ref. 30. One alternative is that the data are more representative of the *small-X* behavior, and that a bend or cusp is not visible because $\mu$ is close to unity and the data have some scatter. The absence of a significant bend in the data may be related to the value of $\Sigma'(0)$. Further discussion of the rationale for assuming the data to be representative of the small-$X$ regime can be found in ref. 29.

Figure 4 illustrates a comparison of the small-$X$ linear behavior predicted by (5.10) with the simulation data of ref. 5. Aside from the vertical offset, the agreement is quite favorable, and from Fig. 5 it appears that the bending generally lies within the scatter of the data. The intercept of the offset curve $\Sigma(0) = 0.56$ is less than, and slightly outside, the value quoted in ref. 5. In these figures, the expression (5.10) was scaled with a factor $b$

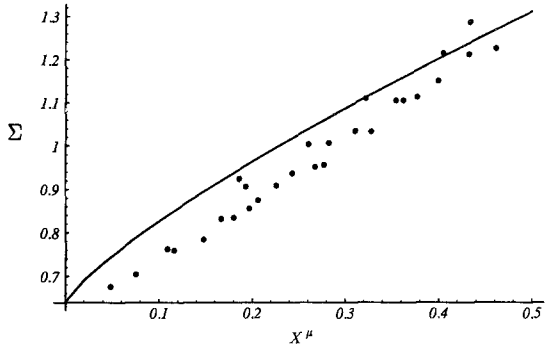


Fig. 4. Comparison of the small-$X$ linear approximation to $\Sigma$ with the simulation data of ref. 5.

of Eq. (5.2) that follows from a $\sigma_0 = 1.78$ for the simulation. An additional factor of $2^{1/\nu d}$ also arises because the system of the simulation has $2L^d$ sites. The amplitude $\sigma_0$ appropriate to the bcc lattice was estimated from the sc lattice result by the relation

$$\sigma_0^{\text{bcc}} = \sigma_0^{\text{sc}} \left[ \frac{\xi_0^{(\pm)\text{sc}}}{\xi_0^{(\pm)\text{bcc}}} \right]^2 \tag{5.14}$$

where $\xi_0^{(\pm)}$ are the correlation length amplitudes for the respective lattices.[31] The value of $\sigma_0^{\text{sc}} = 1.54$ used corresponds to that found from the curve in Fig. 4.

The form of the scaling function when $X \gg 1$ is now considered. It is generally expected that $Y$ should decay exponentially in this regime. This is equivalent to the statement that the ratio of the partition functions must

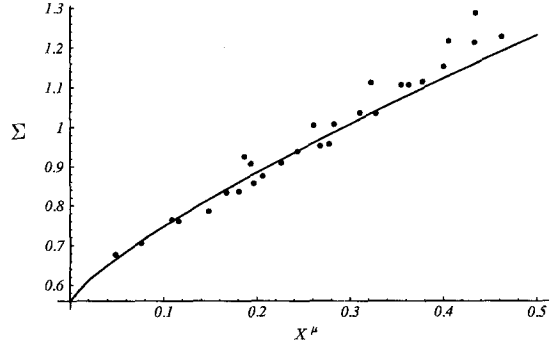


Fig. 5. Comparison of the vertically offset curve of Fig. 5 with the data of ref. 5. The intercept of the offset curve corresponds to $\Sigma(0) = 0.56$.

tend to unity to within exponentially small corrections. This is indeed the case provided spurious higher-order terms arising from the $m$ integration are eliminated. This is an instance in which the results following from the unchecked exact integration over $m$ can even be *qualitatively* incorrect. It follows that[29]

$$\Sigma \simeq \frac{2X^{\mu/2}e^{-X^{\nu}}}{(2\pi)^{3/2}} \tag{5.15}$$

which is essentially obtained from the ratio of the determinants with differing boundary conditions. At the present time, there does not appear to be any simulation data with which to compare this result.

## 5.2. Four Dimensions

Consider now the behavior at four dimensions. Here logarithmic corrections to mean field behavior are expected. For example, the infinite-system surface tension should behave as

$$\sigma \sim \sigma_0 |t|^{3/2} |\ln(-t)|^{1/2} \tag{5.16}$$

For the finite system, below the critical point with $|X| \gg 1$, the behavior of $\Sigma$ is analogous to (5.3) and found to be

$$\Sigma \simeq \sigma_0 |X|^{3/2} - \tfrac{3}{4} \ln(\sigma_0^{2/3} |X|) + C \tag{5.17}$$

where $C$ is given by (5.6) and

$$\tau = -2t \tag{5.18}$$

$$X = \frac{L^2\tau}{2} |\ln \tau|^{1/3} \tag{5.19}$$

$$\sigma_0 \equiv \left(\frac{24K_4}{u}\right)^{1/2} \tag{5.20}$$

In (5.17) terms involving a double logarithm of $t$ are not intended to be taken seriously. A possible approach to demonstrating the presence of logarithmic corrections would be to observe how well the data "scale" with argument $X$. However, due to the logarithmic subdominant contribution, such an approach may at first appear problematic. There may be effects similar to those which made a precise determination of $\sigma_0$ in three dimensions difficult. Analysis of the form (5.17), however, reveals that the

presence of *some* logarithmic factor in $X$ has in general a significantly greater effect than the logarithmic subdominant contribution. It should thus be possible to observe some form of logarithmic corrections, though the precise power of the logarithm may be obscured.

Recently, Münster[32] has studied the finite-size behavior of the energy splitting between symmetric and antisymmetric states of a double well. This so-called "vacuum tunneling energy" is related to the surface tension in essentially the same way as the inverse of the correlation length in a slab geometry. The results of ref. 32 have been found to be in good agreement with some recent four-dimensional numerical simulation data.[33, 34] In particular, a logarithmic factor related to and in accord with that appearing in (5.17) is found to be consistent with the data. The results of this article differ slightly from those of ref. 32 due to the quantities and geometry considered. In particular, there is a discrepancy of a factor $\ln(L/2)$ in addition to different leading exponential corrections to $\Sigma$. With slight modifications, however,[29] the present results may be used to calculate the energy splitting, and yield results in agreement with ref. 32.

The signature of logarithmic behavior can also be found in the vicinity of the bulk critical point. Provided that $L$ is large enough for logarithmic behavior to be present, that is,

$$L \gg e^{2/(3K_4 u)} \tag{5.21}$$

$\Sigma(0)$, though dependent on $L$, is independent of the original coupling $u$. It is found that

$$\Sigma(0) \simeq \frac{1}{4}\ln(\ln L) + 0.21 - \frac{0.43}{(\ln L)^{1/2}} \tag{5.22}$$

which thus should be *universal*. Unfortunately, verification of this form may be difficult due to the presence of the logarithms.

The behavior very close to the critical point is predicted to be

$$\Sigma \simeq \Sigma(0) - \frac{0.85 t L^2 (\ln L)^{1/6}}{u^{1/3}} \tag{5.23}$$

while well above it

$$\Sigma \simeq \frac{2}{(2\pi)^{3/2}} X^{3/4} e^{-X^{1/2}} \tag{5.24}$$

where now

$$X = \frac{L\sqrt{t}}{\frac{3}{8} u K_4 \ln^2(1/t)} \tag{5.25}$$

Notice that close to the critical point, unlike the behavior below four dimensions, a different form of variable enters the free energy. As with the large-$X$ regime, one approach would be to observe the scaling of the data. Though in this regime subdominant parts to the free energy are absent, the fact that $\Sigma(0)$ is $L$ dependent may obscure the determination of the "scaling" variable. This problem might be overcome if the $L$-dependent behavior at the critical point is subtracted off. While the above linear form is representative of the data only for $X \ll 1$, the same form of scaling variable should be applicable when $\Sigma$ deviates from linearity, so long as $X \sim 1$.

## 6. CONCLUDING REMARKS

In this article the techniques developed in refs. 2 and 3 are utilized to determine the finite-size behavior of the surface tension. The most direct approach *naturally* gives rise to a single smooth curve for the scaling function. This curve, however, is not presented, as it follows from a method which is inconsistent in principle. Instead, results are reported that correspond to an approach which extracts contributions that are consistent with the order of the entire calculation. Though the analysis is complicated by the presence of elliptic functions, the analytic results quoted do not require recourse to such functions. It is only necessary to understand the limiting behavior of the profile, lowest modes, and the coupling dependence of various quantities.

In three dimensions, the results for the behavior near the critical point are generally in good agreement with the simulation data. This comparison, however, is based on the assumption that the data of ref. 5 are actually representative of the small- rather than large-$X$ behavior of the scaling function. For large $|X|$ below the critical point, the leading subdominant contribution to the interfacial tension is found to be logarithmic. Though the value of the logarithmic prefactor is slightly outside the actual range of that quoted in the simulations, it is believed to be consistent with those results. Above the critical point, the scaling function is found to decay exponentially provided that the higher-order terms are eliminated.

The expected form of the results in four dimensions has been reported. The approach advocated for identifying the logarithmic behavior is to observe how well the data may be collapsed onto a curve by an appropriate choice of scaling variable. However, when applied to the regime below the critical point where $|X| \gg 1$, it is possible that finite-size effects may obscure the precise power of the logarithm. The form of these subdominant finite-size corrections is similar to that found in three dimensions. While the prefactor to the logarithm is consistent with numerical

data of a system with slab geometry, it would also be of interest to observe how data in a four-dimensional cubic system behave. Consideration of the free energy in the vicinity of the critical point should also reveal the presence of logarithmic corrections. At the critical point, it is also found that the free energy depends on the system size, but is independent of the nonuniversal coupling. Direct comparison of this quantity with the simulation data is thus possible.

## APPENDIX

First we discuss some aspects of the fluctuation operator

$$-\frac{d^2}{dz^2}+\frac{u}{2}\langle\bar{\phi}^2\rangle+t-\lambda \tag{A.1}$$

for the nonuniform system; further details can be found in ref. 29. The modulus $k$ and associated correlation length $\xi$ that appear in (A.1) are those corresponding to the average $\langle m^2\rangle_a$. Rescaling $z$ by $\xi$ leads to consideration of the operator

$$-\frac{d^2}{dy^2}+6k^2\,\mathrm{sn}^2(y)\equiv\Omega \tag{A.2}$$

on the interval $[-K, K]$. Regarding this entity, Hermite[36] has studied the so called Lamé equation of order 2

$$\Omega\psi\equiv\mathscr{E}\psi \tag{A.3}$$

in some detail. With antiperiodic boundary conditions on the interval $[-K, K]$ the two lowest eigenstates and corresponding eigenvalues are

$$\psi_0=\mathrm{cn}\ y\ \mathrm{dn}\ y, \qquad \mathscr{E}=1+k^2 \tag{A.4}$$

$$\psi_1=\mathrm{sn}\ y\ \mathrm{dn}\ y, \qquad \mathscr{E}=1+4k^2 \tag{A.5}$$

and are shown in Fig. 6. The functions $\psi_0$ and $\psi_1$, respectively, correspond to the translation and breathing modes. They go over to the two bound states in the thermodynamic ($k\to 1$) limit and become degenerate in the strong finite-size ($k\to 0$) limit. Notice that the breathing mode and the profile always have nonzero overlap, and the functional forms become identical for zero modulus. It is possible to write down the general solution to Eq. (A.3). Though there are several forms, an especially useful one involves

$$\psi_{\mathscr{E}}=\frac{d}{dy}\left[e^{\rho y}\frac{H(y+\omega)}{\Theta(y)}\right] \tag{A.6}$$

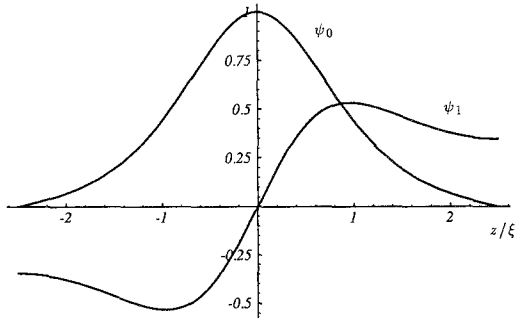


Fig. 6. The translation and breathing modes, denoted respectively by $\psi_0$ and $\psi_1$, that correspond to $L/\xi = 5$.

where $\mathscr{E}$ is to be substituted for $\lambda$ in (4.44), and $\rho$ and $\omega$ are given by the same expressions as in (4.42), (4.44). The functions $H$ and $\Theta$ are Jacobi theta functions and are related to the standard theta functions by (e.g., ref. 35)

$$H(x) = \vartheta_1\left(\frac{\pi x}{2K}\right) \tag{A.7}$$

$$\Theta(x) = \vartheta_4\left(\frac{\pi x}{2K}\right) \tag{A.8}$$

The function $\Theta$ should not be confused with that appearing in Section 4. Because the potential in (A.3) is reflection invariant, if $\psi(y)$ is a solution, so is $\psi(-y)$. Provided these two functions are linearly independent, which is the case unless $\rho$ vanishes, the general solution is

$$f_{\mathscr{E}} = c_1 \psi_{\mathscr{E}}(y) + c_2 \psi_{\mathscr{E}}(-y) \tag{A.9}$$

The Fredholm determinant was calculated[29] by a method which utilizes the fact that if an analytic function $\Delta(\lambda)$ is found that has zeros at the eigenvalues of the operator, then $\Delta$ is proportional to the determinant. In practice, actually the better defined ratio of determinants was considered. The calculation of this quantity was essential to ascertain the behavior that resulted from the exact integration over $m$. However, once this approach was modified, it was found to be no longer necessary to consider the expression for the determinant, which is valid for general modulus $k$.

The term $(\bar{\phi}_a, G_a \bar{\phi}_a)$ found in (4.16) is now discussed. If an exact integration over $m$ were necessary, then in principle a closed-form result for this quantity also would be required. It is in fact possible to find an

expression for $G_a$ by solving the appropriate boundary value problem. However, the quantity $(\bar{\phi}_a, G_a\bar{\phi}_a)$ unlike the determinant, does not take on a form amenable to simple and accurate numerical methods. Thus, when the behavior resulting from the exact integration was considered, an approximation for this quantity was employed:

$$(\bar{\phi}_a, G_a\bar{\phi}_a) \simeq \frac{(\bar{\phi}_a, \hat{\psi}_1)^2}{\lambda_b} - \frac{(\bar{\phi}_a, \bar{\phi}_a) - (\bar{\phi}_a, \hat{\psi}_1)^2}{\lambda_2} \tag{A.10}$$

where

$$\hat{\psi}_1 = \frac{\psi_1}{\|\psi_1\|} \tag{A.11}$$

$$\lambda_b = \frac{1}{\xi^2}(4k^2 + 1) + t \tag{A.12}$$

and $\lambda_2$ is the next eigenvalue following $\lambda_b$. Analysis shows that this approximation becomes exact when the modulus $k$ is either very small or close to unity. It also shows that the problems associated with the exact integration will persist even in the absence of the approximation.

When the exact integration over $m$ is abandoned, a closed-form result for this quantity is unnecessary. All that is required are the limiting forms when the modulus approaches zero or unity. Regarding the first limit, recall that the breathing mode and profile become identical up to an amplitude as the modulus approaches zero. In this limit the spectral decomposition of $(\bar{\phi}_a, G_a\bar{\phi}_a)$ reduces to the single term

$$(\bar{\phi}_a, G_a\bar{\phi}_a) \to \frac{(\bar{\phi}_a, \hat{\psi}_1)^2}{\lambda_b} \tag{A.13}$$

The result corresponding to the other limit $k \sim 1$ is

$$(\bar{\phi}_a, G_a\bar{\phi}_a) \to \frac{3L^d}{g}\left(1 - \frac{\xi}{L}\right) \tag{A.14}$$

which follows from the forms of the profile and correlation function appropriate to an infinite system. Analysis reveals that, to order $u$, all algebraically decaying terms contributing to $\Sigma$ cancel.

It was noted in Section 4 that $\mathscr{J}$ involved an "external" factor of $|m|$, Eq. (4.16). While this might appear odd in that configurations with small $m$ have vanishingly small weight, it is of the expected form. For example, consider the behavior close to the critical point where the integration over

profiles reduces to the integration over the breathing mode. In this limit, the two lowest modes take the form

$$\psi_0 \simeq \cos\left(\frac{\pi z}{L}\right) \tag{A.15}$$

$$\psi_1 \simeq \sin\left(\frac{\pi z}{L}\right) \tag{A.16}$$

The contribution to the fluctuation $\sigma$ is thus

$$\sigma \sim \left(\frac{2}{L^d}\right)^{1/2}\left[A_0 \cos\left(\frac{\pi z}{L}\right) + A_1 \sin\left(\frac{\pi z}{L}\right)\right] \tag{A.17}$$

Changing to amplitude and phase coordinates defined by

$$m^2 = \frac{2}{L^d}(A_0^2 + A_1^2) \tag{A.18}$$

$$z_0 = \frac{L}{\pi}\tan^{-1}\left(\frac{A_0}{A_1}\right) \tag{A.19}$$

it follows that

$$\frac{dA_0\, dA_1}{2\pi} = \frac{dm\, dz_0\, |m| L^{d-1}}{4} \tag{A.20}$$

This is consistent with the expression given by the small modulus limit of $\mathscr{J}$ once the factor $\langle G_a \rangle^{1/2}$ has been used to cancel the breathing mode eigenvalue from the determinant.

Finally, consider the origin of the logarithmic factor found in (5.3). The factors of $L$ mentioned in the following are those multiplying the partition functions. Inspection of the form of the Jacobian factor for the antiperiodic system (4.16) reveals that

$$j \sim L^{*d/2} L^{*(d-1)/2} \tag{A.21}$$

while that for the periodic system (2.7) is $L^{*d/2}$. The $m$ integration contributes a factor $L^{*-d/2}$ for both the one- and two-phase systems. For the antiperiodic system there are two additional factors, which cancel, one of $L^*$ from the integration over the profile center, and another of $1/L^*$ arising from the lattice sum for the capillary modes. Putting these results together, it follows that the overall multiplicative factor to the partition function ratio is

$$\frac{Z_a}{Z_p} \sim L^{*(d-1)/2} \tag{A.22}$$

Hence, the logarithmic factor appearing in $\Sigma$ is

$$-\frac{d-1}{2}\ln L^* \sim -\frac{\mu}{2}\ln |X| \tag{A.23}$$

since in this limit

$$L^* = e^{-l^*}L \sim |t|^{\nu} L = |X|^{\nu} \tag{A.24}$$

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