

FINAL EXAM Spring 2011
TFY4235/FY8904 Computational Physics

This exam is published on Friday, May 13, 2011 at 09:00 hours. The solutions should be mailed to me at Alex.Hansen@ntnu.no on Monday, May 16 at 23:00 hours at the latest. There are no constraints on any aids you may want to use in connection with this exam, including discussing it with anybody. Do collaborate on the development of the programs, but write your own code. The final report you will have to write yourself. Please attach your programs as appendices to the report. The report may be written in either Norwegian (either variation) or in English. Please use name rather than candidate number on the report. The reports should be in PDF format and consist of a single file.

This year's topic is *line tension* in the two-dimensional Ising model. We will test a new numerical method for calculating this quantity.

The Ising model implemented on a square lattice has the Hamiltonian (energy function)

$$H = -\frac{J}{2} \sum_{\langle \vec{m}, \vec{n} \rangle} \sigma_{\vec{m}} \sigma_{\vec{n}} , \quad (1)$$

where $\sigma_{\vec{m}} = \pm 1$ is the spin at node $\vec{m}$ and the sum over $\langle \vec{m}, \vec{n} \rangle$ runs over all nearest neighbors. Hence, for each $\vec{m}$, we sum over its four nearest neighbors $\vec{n}$. This leads to double counting, explaining the factor 1/2. The coupling strength is J . In the following, we set $J = 1$.

We now describe the square lattice. We orient it with respect to a cartesian coordinate system (x, y) so that the principal axes coincide with the axes of the coordinate system. Hence, the node address $\vec{m}$ can be written $\vec{m} = (i_m, j_m)$, where i_m is the coordinate of $\vec{m}$ along the x axis and j_m is the coordinate of $\vec{m}$ along the y axis. We limit the size of the lattice to the two intervals $1 \leq i_m \leq N_x$ and $1 \leq j_m \leq N_y$.

We assume in the following periodic boundary conditions in the y direction. That is, the lattice is rolled into a tube so that the $j_m = 1$ and $j_m = N_y$ rows are next to each other. We will in a moment discuss the boundary conditions in the x direction.

In 1984, Mon and Jasnow (Phys. Rev. A, **30**, 670 (1984)) proposed an algorithm to measure the line tension in the Ising model. The line tension is the free energy associated

with the boundaries between islands of up and down spins. Mon and Jasnow proposed the following: Prepare *two* lattices as described above. In both of them, add a row in the y direction with $i_m = 0$. Along this row, all spins are *fixed* (i.e., do not change) and set to the value $\sigma_{(0,j)} = +1$. Next, in one of the lattices add a row in the y direction at $i_m = N_x + 1$ where the spins are fixed, $\sigma_{(N_x+1,j)} = +1$, whereas in the other lattice, the extra row in $(N_x + 1, j)$ has fixed spins with value $\sigma_{(N_x+1,j)} = -1$. The hamiltonian, defined in Eq. (1), for the first lattice we denote H_{++} , whereas the hamiltonian for the second lattice, we denote H_{+-} .

We may now define the free energy associated with the line tension in the Ising model. If F_{++} is the free energy associated with the $++$ lattice and $+-$ the free energy associated with the $+-$ lattice, the surface tension free energy $i\tau$ is

$$N_y \tau = F_{+-} - F_{++} . \quad (2)$$

This is easy to understand intuitively since in the $+-$ lattice there *must* be an interface at zero temperature T forced into existence by the boundary conditions in the x direction.

The free energies F_{++} and F_{+-} are related to the partition functions and hence the hamiltonians through the expressions

$$e^{-F_{++}/k_B T} = Z_{++} = \sum_{conf.} e^{-H_{++}/k_B T} , \quad (3)$$

and

$$e^{-F_{+-}/k_B T} = Z_{+-} = \sum_{conf.} e^{-H_{+-}/k_B T} . \quad (4)$$

The sum runs over all possible spin configurations. In the following, we use units so that the Boltzmann constant $k_B = 1$.

Combining Eq. (2) with Eqs. (3) and (4) gives

$$\tau = -\frac{T}{N_y} \ln \frac{Z_{+-}}{Z_{++}} . \quad (5)$$

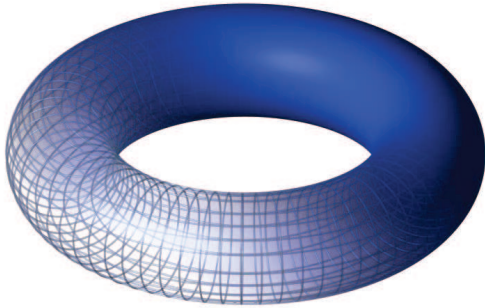
The ratio between the two partition functions may be written (and this is main observation of Mon and Jasnow)

$$\frac{Z_{+-}}{Z_{++}} = \frac{\sum_{conf.} e^{-(H_{+-} - H_{++})/T} e^{-H_{++}/T}}{Z_{++}} = \langle e^{-(H_{+-} - H_{++})/T} \rangle_{++} . \quad (6)$$

That is, the ratio Z_{+-}/Z_{++} equals average of the quantity $\exp[-(H_{+-} - H_{++})/T]$ in the system governed by the H_{++} hamiltonian.

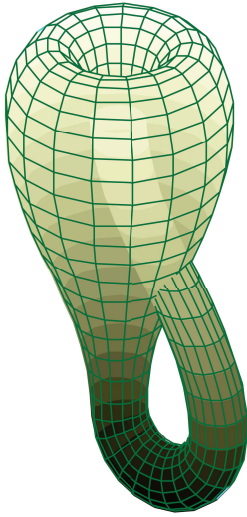
The quantity $\langle \exp[-(H_{+-} - H_{++})/T] \rangle_{++}$ we sample numerically using the *Metropolis Monte Carlo algorithm*. That is, we use the Boltzmann weight $\exp[-H_{++}/T]$ for the probability distribution.

So far the Mon and Jasnow algorithm for calculating τ . Here is the *new* idea for this exam. The Mon and Jasnow algorithm uses two fixed boundary layers at $i_m = 0$ and $i_m = N_x + 1$. These two fixed boundary conditions will disturb the calculation for small lattice sizes and getting rid of them would be an improvement. We therefore introduce the following algorithm. Use two lattices as in the Mon and Jasnow algorithm. In one of the lattices, use *periodic boundary conditions* also in the x direction. This means that the $i_m = 1$ row is neighbor to the $i_m = N_x$ row in the x direction. Hence, the lattice forms a *torus*, see the figure below.

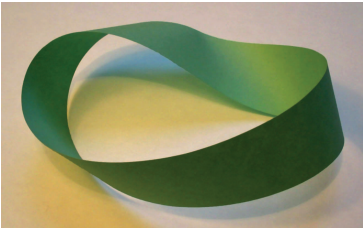


We call the hamiltonian, Eq. (1), for this system H_t .

The second lattice, we implement on a *Klein bottle*, the structure shown here:



This curious structure has only one side. If we cut out a ribbon in the horizontal direction, the ribbon will form an annulus (ring). However, if we cut out a ribbon in the vertical direction, it will form a *Möbius strip* as shown here:



We call the hamiltonian, Eq. (1), for the Klein bottle H_k .

At temperature $T = 0$, there will be an interface in the Klein bottle system but not in the torus system. We may therefore define the free energy associated with the line tension

$$N_y \tau = F_k - F_t . \quad (7)$$

where the subscripts k and t refer to the Klein bottle system and the torus system respectively. By following step by step the arguments leading up to Eqs. (5) and (6), we find

$$\tau = -\frac{T}{N_y} \ln \langle e^{-(H_k - H_t)/T} \rangle_t , \quad (8)$$

where the average $\langle \dots \rangle_t$ is calculated through Metropolis Monte Carlo using the torus system.

It sounds very difficult to implement the Klein bottle boundary conditions. It is not. Just connect the node at $j_m = j$ on the $i_m = 1$ row with the node at $j_m = N_y + 1 - j$ on $i_m = N_x$ row through a *reversed sign* in the coupling constant in the hamiltonian. Hence, $H_k = \dots - \sigma_{1,2} \sigma_{2,2} + \sigma_{N_x, iN_y+1-2} \sigma_{1,2} - \dots$. This is all.

It is the aim of this exam to test whether the Klein bottle construction works for calculating the line tension free energy. It has never been considered before and I hope it works, but there is no guarantee.

The Ising model on the square lattice has a critical point at a temperature $T = T_c = 2/\ln(1 + \sqrt{2}) \approx 2.2691 \dots$. Below this temperature, the line tension free energy is different from zero, whereas above this temperature, it is zero. If we introduce the reduced temperature

$$t = \frac{T_c - T}{T_c} , \quad (9)$$

the line tension free energy may be given the form

$$\tau = \tau_0 t^\mu \Sigma \left(N_y^{1/\nu} t \right) , \quad (10)$$

for temperatures T below T_c . According to Onsager's famous exact solution of the Ising model on the square lattice $\mu = 1$, $\nu = 1$ and $\tau_0 = 3.99 \dots$. Here, $\Sigma(X)$ is a *scaling function* that approaches 1 as $X \rightarrow \infty$ and $\Sigma(X) \sim X^{-\mu}$ as $X \rightarrow 0$.

Plot the line tension τ as a function of temperature T and verify that there is a phase transition at $T = T_c$. Do this for different N_y (and let $N_y = N_x$ so that you change the linear size in both the x and y direction simultaneously). You should see the transition becoming sharper for increasing N_y . If you for $T = T_c$ ($t = 0$) show τ *vs.* N_y in log-log plot, you should get a straight line with slope $-\mu/\nu = -1$ (why?). Show this numerically. Next, for a number of different values of t , plot $t^{-\mu}\tau$ as a function of $1/(N_y^{1/\nu}t)$ where you vary N_y . You should find that all the data fall on a single curve that crosses the y axis at the value $\tau_0 = 3.99\dots$. Show this numerically.

If for some reason, the Klein bottle construction should give trouble, do these plots for the Mon and Jasnow system where we know it works.

Good luck!

Direct calculation of interfacial tension for lattice models by the Monte Carlo method

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We present a novel application of Monte Carlo sampling techniques for the direct evaluation of the interfacial tension that is applicable over a wide range of system sizes and temperatures. The results for the two-dimensional Ising model with system size up to 32×32 for temperature at and below T_c have been analyzed within scaling theory. An accurate estimate for the surface-tension amplitude in excellent agreement with Onsager's exact result is obtained.

Despite extensive current interest in the statistical mechanics of surfaces and interfaces,¹ there has not yet appeared a simple Monte Carlo method for the direct evaluation of interfacial tension that is applicable to large systems and over a range of temperatures. Standard thermodynamic integration techniques are very useful far below the critical temperature (T_c), but become difficult to apply near T_c . Recently, an elegant method based on studies of the order-parameter distribution has been introduced by Binder.² The approach appears to be quite successful, but, as was noted,² it is limited to temperatures close to T_c and in system size. In this paper we present a novel extension of Monte Carlo sampling techniques for direct evaluation of the interfacial tension, applicable over a wide range of system size and temperature. This method has been applied to the two-dimensional Ising model for system size up to 32×32 and for temperature at and much below T_c . The results have been analyzed within finite-size scaling assumptions and are in excellent agreement with exact results. The approach and results from this initial application are presented here.

A method for evaluation of the surface tension or its analog is also of interest in field-theoretic applications. A class of ferromagnetic Ising models will allow construction of dual models. As noted, for example, by Brimont, Lebowitz, and Pfister³ the surface tension of the original Ising model relates to the asymptotic behavior of certain spin correlations in the dual model. For $d=3$ the dual is the Ising gauge model⁴ and the surface tension of the "direct" model equals precisely the coefficient of the area-law decay of the Wilson loop.⁴ In $d=2$ the surface tension equals directly the mass gap or inverse correlation length at the dual temperature.

We consider here a nearest-neighbor ferromagnetic Ising model on a square lattice with $N_y \times N_x$ ($N_y = N$, $N_x = N+2$) spins ($\sigma_{ij} = \sigma_{x,y} = \pm 1$) with exchange coupling J at temperature T in zero magnetic field. The Ising system is considered under two sets of boundary conditions, as shown schematically in Fig. 1. Periodic boundary conditions are always taken for the top and bottom edges as shown in Figs. 1(a) and 1(b). The boundary conditions $(++)$ then refer to the situation shown in Fig. 1(a) in which the first and last columns of spins are fixed with value $\sigma = +1$. The alterna-

tive set of boundary conditions $(+-)$ then refer to the situation of Fig. 1(b). For $T < T_c$ the interfacial tension τ is taken to be³ the difference of free energies

$$\tau = -k_B T / N \ln \frac{Z_{+-}}{Z_{++}} \quad (\text{as } N \rightarrow \infty), \quad (1)$$

where Z_{+-} and Z_{++} are the partition functions for the $N \times (N+2)$ lattice systems described above. Equation (1) may be rewritten in a form more suitable for Monte Carlo sampling as

$$\begin{aligned} N\tau_N &= -k_B T \ln \langle \exp[-(1/k_B T)(\mathcal{H}_{+-} - \mathcal{H}_{++})] \rangle_{++} \\ &= -k_B T \ln \langle \exp[-(2J/k_B T)m_s] \rangle_{++}, \end{aligned} \quad (2)$$

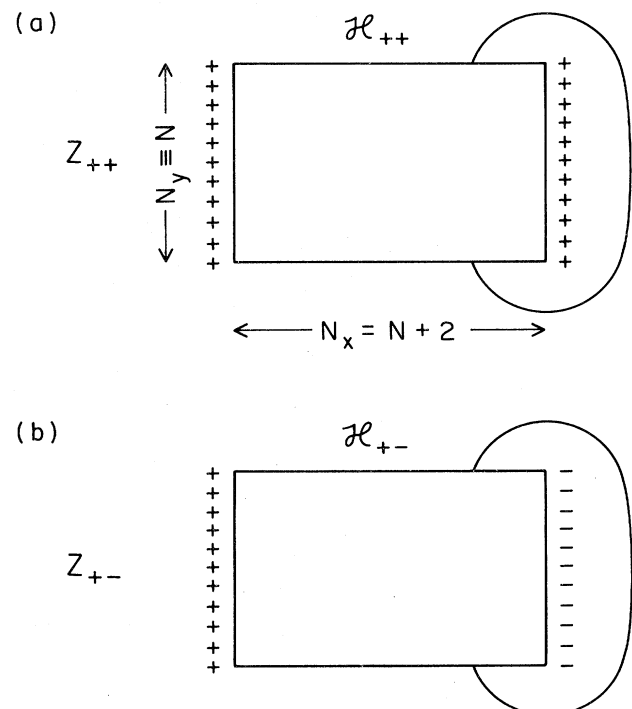


FIG. 1. Boundary conditions for $\mathcal{H}_{++}$ and $\mathcal{H}_{+-}$.

where $m_s = \sum_{i=1}^N \sigma_{N+1,i}$ is the magnetization of the layer adjacent to the fixed "all minus" layer shown in Fig. 1(b), and the ensemble average $\langle \rangle_{++}$ is generated by the Hamiltonian $\mathcal{H}_{++}$ defined by the $(++)$ boundary condition. The interfacial tension can then be evaluated as an ensemble average.

This formulation represents direct sampling of the difference in free energy between two systems by weighting configurations generated by $(++)$ ensemble. Such a method is useful only when there is sufficient overlap in the configurations sampled by the two ensembles. This then limits its usefulness to very small systems and near T_c .⁵ To circumvent this difficulty, observe that Eq. (2) can be rewritten by considering

$$\langle \exp[-(1/k_B T)(\mathcal{H}_{+-} - \mathcal{H}_{++})] \rangle_{++} = \frac{\langle \exp[-(1/k_B T)(\mathcal{H}_{+-} - \mathcal{H}')] \rangle_{\mathcal{H}'}}{\langle \exp[-(1/k_B T)(\mathcal{H}_{++} - \mathcal{H}')] \rangle_{\mathcal{H}'}} , \quad (3)$$

where now the ensemble is generated by some Hamiltonian $\mathcal{H}'$ (defined by some boundary conditions) which can be chosen such that overlap of configurations generated by $\mathcal{H}'$ with those of $\mathcal{H}_{+-}$ and $\mathcal{H}_{++}$ is a maximum. Observe that both ensemble averages on the right-hand side of Eq. (3) can be evaluated simultaneously within one single ensemble generated by $\mathcal{H}'$. Although only one stage is used, this formulation is in the spirit of the well-known multistage sampling technique.⁶ Its application to the evaluation of the interfacial tension is novel and, as shall be shown below, can be an efficient method for calculating the interfacial tension, even in large systems and well below T_c .

The optimum choice for $\mathcal{H}'$ is found by considering boundary conditions which yield sampling, with comparable frequency, of configurations generated by both $\mathcal{H}_{+-}$ and $\mathcal{H}_{++}$. One such boundary condition which leads to rather efficient sampling is a hybrid boundary condition. The spins on one edge are fixed to be all "+", say, while the spins on the other edge are fixed to be + or - (with numbers $N_+ + N_- = N$) in an alternating sequence (see Fig. 2). Although this kind of boundary condition is unbiased with respect to $\mathcal{H}_{+-}$ and $\mathcal{H}_{++}$, configurations with an interface (i.e., those with $\mathcal{H}_{+-}$) occur with probability reduced by $\sim \exp(-\tau N/k_B T)$, where τ is the interfacial tension. This becomes important at low temperature and for large

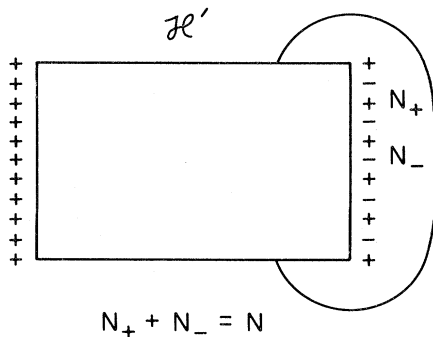


FIG. 2. Boundary conditions for $\mathcal{H}'$ of Eq. (3). N_+ is the number of sites fixed in the + configuration and N_- is the number of sites fixed in the - configuration. Note that N_+ need not equal N_- .

systems, where $\tau N/k_B T$ is large. This difficulty can be reduced in part by choosing on the mixed edge the number of "+" and "-" spins, N_+ and N_- , such that $N_+ < N_-$ which (then) favors sampling more configurations with an interface. We note that the choice of boundary condition (or $\mathcal{H}'$) should only affect the sampling efficiency or the rate of convergence. It does not affect the final results, if sufficiently long sampling is employed to ensure equilibrium. Furthermore, the boundary condition considered here need not be optimum and better choices may exist. However, we have found that for the two-dimensional Ising model, this scheme suffices for size up to $N=32$ with $\leq 10^6$ Monte Carlo steps per site. This represents the largest system considered in a surface-tension computation.

Our results for the interfacial tension of the two-dimensional Ising models is given in Fig. 3. A few low-temperature cases have been considered for the purpose of illustrating that the method works well in that region. Note that there is excellent overall agreement with Onsager's exact result.⁷ By considering a system size N from 2 to 32, for temperatures near and at T_c , we have been able to use the finite-size scaling behavior of the interfacial tension. In analogy with the usual assumptions,⁸ we make a scaling ansatz:

$$\tau = \tau_0 t^\mu \sum(x)$$

with

$$x = c_L N^{1/\nu} t, \quad t = \frac{T_c - T}{T_c} . \quad (4)$$

Here μ and ν are the appropriate critical indices for the interfacial tension and correlation length, respectively, and τ_0 and c_L are nonuniversal constants. The universal scaling function $\sum(x)$ has the asymptotic limits, $\sum(x \rightarrow \infty) = 1$ and $\sum(x \rightarrow 0) \sim x^{-\mu}$. For the two-dimensional Ising model, $\mu = \nu = 1$. The limiting forms of $\sum(x)$ are such that $\tau \sim t^\mu$ in the thermodynamic limit, and that at the bulk critical temperature, $\tau \sim N^{-\mu/\nu} \sim N^{-1}$. The critical temperature $J/k_B T_c = 0.44068 \dots$ is, of course, known exactly; accordingly, a plot of τN vs N at T_c is made in Fig. 4. The asymptotic limit appears to be reached for $N \geq 8$, the results being consistent with $\tau \sim N^{-1}$.

It is of considerable interest to evaluate as precisely as possible a universal ratio involving the surface-tension am-

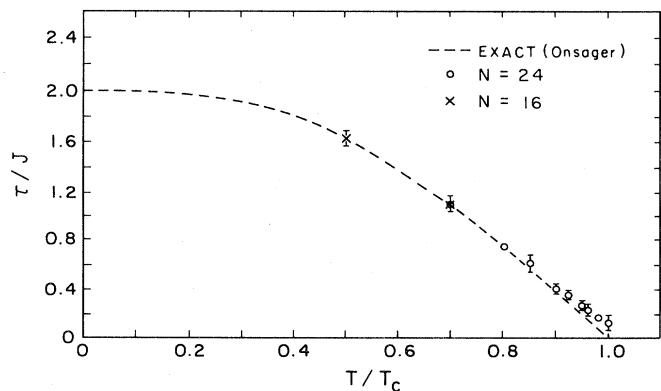


FIG. 3. Comparison of representative Monte Carlo results with exact solution for the infinite system by Onsager (Ref. 6).

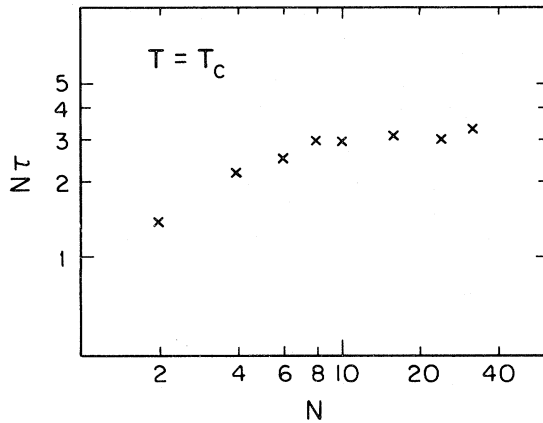


FIG. 4. Finite-size scaling analysis for $T = T_c$ or $t = 0$, for $N = 2$ to 32. Results for $N = 2$ and 4 are exact.

plitude τ_0 . Such information is needed, for example, in discussions of critical wetting.⁹ The simplest relation involves the specific heat, which may be written analogously to (4) as

$$C = \frac{A_0}{\alpha} t^{-\alpha} W(x), \quad (5)$$

with $W(x) \rightarrow 1$ as $x \rightarrow \infty$ (thermodynamic limit) and as usual $W(x) \rightarrow x^\alpha$ as $x \rightarrow 0$. The ratio is, in the thermodynamic limit, given by¹⁰

$$U_\tau = \lim_{\tau \rightarrow 0} \frac{\tau(t)/k_B T_c}{[\alpha^2 C(t)]^{(d-1)/d}} = \frac{\tau_0/k_B T_c}{A_0^{(d-1)/d}}. \quad (6)$$

Unfortunately, a finite-size extrapolation at $T = T_c$ is not sufficient to extract U_τ because subdominant parts of the scaling functions as $x \rightarrow 0$ are required but cannot be determined with the size systems one may realistically treat.

By probing away from but near $T = T_c$ one may plot $\tau t^{-\mu}$ vs $N^{1/\nu} t$. One must reach the scaling limit; according to Eq. (4) the asymptotic value for large $N^{1/\nu} t$ yields τ_0 . This plot is shown for the $d=2$ Ising model in Fig. 5. For size 32×32 (with $t = 0.05$) the value is still about 20% above the exact value. Nonetheless, this represents considerable progress, and larger systems can in principle be considered within this approach. Also shown in Fig. 5 are points corresponding to $t = 0.1$ and 0.2 . The danger of trying to reach the scaling limit (large $tN^{1/\nu}$) by taking too-large values of t is clearly demonstrated. The amplitude A_0 is exactly known in $d=2$, but more generally it would have to be determined from a finite-size analysis as well (off T_c).

Further progress can be made without using excessively large system by considering alternative means of analysis. This is motivated by the following observations. The difficulty with $\Sigma(x)$ is related to its slow approach toward the large x limit of $\Sigma(\infty) = 1$. One may surmise that this is related to the $x \rightarrow 0$ limits where $\Sigma(x \rightarrow 0) \cong Bx^{-\mu}$ diverges. This limiting property incorporates the scaling of the surface tension at $t=0$ which is, $\tau_N(t=0) \cong \tau_0 B c_L^{-\mu} N^{-\mu/\nu}$. Here, c_L is a nonuniversal amplitude related to the correlation length and B is a universal constant. We will consider removing this singular part from $\Sigma(x)$ by adding and subtracting $Bx^{-\mu}$ and introducing $Y(x)$ with $\Sigma(x) = Bx^{-\mu}$

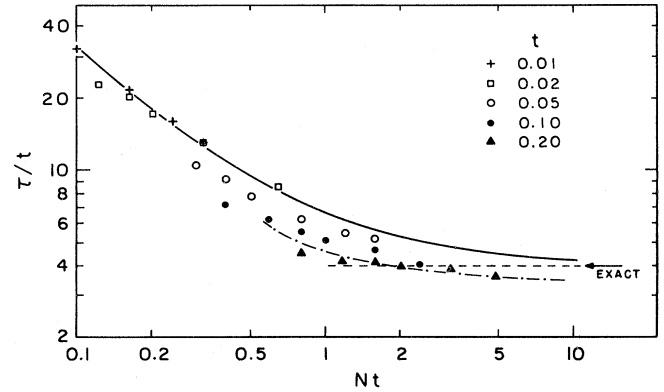


FIG. 5. Finite-size scaling analysis for $T < T_c$ with $N \leq 32$. The ratio τ/t^μ approaches τ_0 in the limit of large x ($N^{1/\nu} t^\mu$). The exact result (Ref. 7) is indicated and the solid line is an extrapolation of data at $t=0.01$ using Eq. (10). The dash-dot line indicates some deviations when using data far from T_c ($t \leq 0.20$).

+ $Y(x)$. The surface-tension expression Eq. (4) becomes

$$\tau_N(t) = \tau_N(t=0) + \tau_0 t^\mu Y(x). \quad (7)$$

The limiting forms are $Y(x) \rightarrow 1$ as $x \rightarrow \infty$, and as $x \rightarrow 0$ with $t \rightarrow 0$, $t^\mu Y(x) \rightarrow 0$. It is sufficient to assume

$$Y(x \rightarrow 0) \cong B' x^{-\mu'} \text{ as } x \rightarrow 0, \quad (8)$$

with $0 \leq \mu' < \mu$ and B' is an additional amplitude, which merely asserts a power law for the subdominant part of the original $\Sigma(x)$. This then suggests considering

$$N^{\mu/\nu} \tau_N(t) = N^{\mu/\nu} \tau_N(t=0) + N^{\mu/\nu} t^\mu \tau_0 Y(x) \quad (9)$$

and a plot of $N^{\mu/\nu} \tau_N(t)$ vs $N^{\mu/\nu} t^\mu$ to obtain τ_0 as the limiting slope with large x . $N^{\mu/\nu} \tau_N(t=0)$ would also be obtained as the intercept by extrapolating back to $x=0$. With this analysis for the data at $t = 0.01$, we found that for $N \geq 16$ ($N^{\mu/\nu} t^\mu \geq 0.16$), $Y(x)$ has reached its large- x limit. We obtain $\tau_0 = 3.96 \pm 0.2$ and $N^{\mu/\nu} \tau_N(t=0) = 2.9 \pm 0.2$. The exact result of Onsager⁷ is $\tau_0 = 3.99 \dots$, and the estimate for $N^{\mu/\nu} \tau_N(t=0)$ from scaling analysis of the data at $t=0$ is 3.0 ± 0.3 . (See Fig. 4.) An "approximant" for $N^{\mu/\nu} t^\mu \geq 0.16$ is then suggested,

$$\begin{aligned} \Sigma(x) &\cong 1 + Bx^{-\mu} \\ &= 1 + 0.7323(N^{1/\nu} t)^{-\mu}, \end{aligned} \quad (10)$$

which is shown as the solid curve in Fig. 5.

Observe that Eq. (10) has the correct large and small x limits. These suggested results are obtained in the finite-size region and may shed some light on the structure of the scaling function in that region. Such information may prove useful for simulations of Ising and other systems.

We have described a method for direct evaluation of interfacial tension which is applicable to large systems at or below T_c . Although for the system sizes and temperatures considered the one-stage formulation suffices, for much larger systems ($N \gg 32$) and lower temperatures, multi-stage extension of Eq. (3) would be necessary, but is straightforward. The important observation is that computational efforts (or number of stages) would only increase roughly linearly with system size or on lowering tempera-

ture. Thus, this method should be a useful technique in the study of interfaces for large systems and in three dimensions where a considerable number of important problems await solution. Preliminary work on the $d=3$ case is encouraging.

David Jasnow is grateful to the National Science Foundation through the Division of Materials Research for support of this work and K. K. Mon is grateful for the support of the National Science Foundation through the Center for Joining of Materials.

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