Direct Monte Carlo Measurement of the Surface Tension in Ising Models

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Abstract

I present a cluster Monte Carlo algorithm that gives direct access to the interface free energy of Ising models. The basic idea is to simulate an ensemble that consists of both configurations with periodic and with antiperiodic boundary conditions. A cluster algorithm is provided that efficiently updates this joint ensemble. The interface tension is obtained from the ratio of configurations with periodic and antiperiodic boundary conditions, respectively. The method is tested for the 3-dimensional Ising model.
1 Introduction

The interfaces of 2D and 3D Ising models at temperatures below the bulk critical temperature $T_c$ have been studied as models of interfaces separating coexisting phases of fluids. There are also relations to lattice gauge theory: The surface tension of the 3D Ising model is equal to the string tension of the 3D $Z_2$ gauge model which is dual to the 3D Ising model.

While in the 2D case a number of exact results have been obtained, Monte Carlo simulations play a major role in the study of 3D systems. Recently a number of simulations employing various methods have been performed to determine the surface tension of 3D and 4D Ising models [1, 2, 3, 4, 5, 6], while in ref. [7] the string tension of the 3D $Z_2$ gauge model is studied.

As the temperature $T$ increases towards the critical temperature $T_c$, the reduced surface tension

$$\sigma = \sigma_0 t^\mu,$$

where $t = (T_c - T)/T_c$, and $\sigma_0$ is the critical amplitude of the reduced interface tension. Widoms scaling law [8, 9]

$$\mu = (D - 1) \nu$$

relates the universal critical exponent $\mu$ to the critical exponent of the correlation length

$$\xi = \xi_0 t^{-\nu}.$$

In a recent Monte Carlo Renormalization Group study of the 3D Ising model on a simple cubic lattice [10] $\beta_c = 0.221652(4)$ and $\nu = 0.624(2)$ have been obtained, while $\epsilon$-expansion predicts $\nu = 0.630(2)$ [1]. The experimental [12, 13, 14, 15] value for $\mu$ is $\mu = 1.26(1)$, consistent with Widoms scaling law. Ratios of critical amplitudes should also be universal due to the scaling hypothesis [16, 17]. Experimental results for various binary systems are consistent with

$$R_+ = \sigma_0 (\xi_0^+)^2 = 0.386$$

[15], where $\xi_0^+$ is the critical correlation length amplitude in the high temperature phase.

An interesting question is the relation of the surface tension with the correlation length of a system with cylindrical geometry, i.e. a system on a lattice with extension $L \times L \times T$, where $T \gg L$. Recently, Borgs and Imbrie [18] gave an exact derivation of the finite size behaviour of the correlation length of discrete spin systems in a cylindrical geometry. They claim that for sufficiently large couplings the properties of the system are given by an effective 1D model, where the diagonal parts of the transfer matrix are given by the free energies of the pure phases, while the off diagonal elements are
determined by the surface tensions between the different phases. For the 3D Ising model this leads to the relation

$$\xi_L = \exp(\sigma L^2).$$

(5)

A semiclassical instanton calculation \[19\] however predicts

$$\xi_L = c \exp(\sigma L^2),$$

(6)

where $c$ depends on the temperature and is not equal to 1.

In order to understand this discrepancy I compared the correlation length of an 1D Ising model with

$$2\beta_{\text{eff}} = F_s,$$

(7)

where $F_s$ is the reduced surface free energy, with the correlation length measured in ref. \[9\] for 3D Ising cylinders.

The correlation length $\xi$ of a 1D Ising model is given by

$$\xi = \frac{1}{\ln((1 + v)/(1 - v))},$$

(8)

where $v = \exp(-2\beta)$. For large $\beta$ one gets approximately

$$\xi \approx \frac{1}{2v}.$$  

(9)

This paper is organized as follows. First I explain the model with periodic and antiperiodic boundary conditions. I discuss how one can get the surface tension from observables of a system which includes the boundary conditions as dynamical variables. Then I present a cluster algorithm which is suitable for the simulation of such a system. Finally the numerical results will be given and compared with recent Monte Carlo studies employing other methods.

2 The Model

I consider a simple cubic lattice with extension $L$ in $x$- and $y$-direction and with extension $T$ in $z$-direction. The uppermost layer of the lattice is regarded as the lower neighbor plane of the lowermost plane. An analog identification is done for the other two lattice directions. The Ising model is defined by the Hamiltonian

$$H(s, b.c.) = - \sum_{<ij>} J_{<ij>} s_i s_j.$$  

(10)

When periodic (p.) boundary conditions (b.c.) are employed, then $J_{<ij>} = 1$ for all nearest neighbor pairs. When antiperiodic (a.p.) boundary conditions are employed, then $J_{<ij>} = -1$ for bonds $<ij>$ connecting the lowermost and uppermost plane of the lattice, while all other nearest neighbor pairs keep $J_{<ij>} = 1$. 

3
3 The Surface Tension

I consider a system that allows both periodic and antiperiodic boundary conditions. The partition function of this system is given by

\[ Z = \sum_{b.c.} \sum_{s_i=\pm 1} \exp(-\beta H(s, b.c.)). \]  \hspace{1cm} (11)

The fraction of configurations with antiperiodic boundary conditions is given by the ratio \( \frac{Z_{a.p.}}{Z} \),

\[
\frac{Z_{a.p.}}{Z} = \frac{\sum_{s_i=\pm 1} \exp(-\beta H(s, a.p.))}{\sum_{b.c.} \sum_{s_i=\pm 1} \exp(-\beta H(s, b.c.))\delta_{b.c.,a.p.}} = \langle \delta_{b.c.,a.p.} \rangle . \hspace{1cm} (12)
\]

An analogous result can be found for periodic boundary conditions. Now we can express the ratio \( \frac{Z_{a.p.}}{Z_{p.}} \) as a ratio of observables in this system.

\[
\frac{Z_{a.p.}}{Z_{p.}} = \frac{\sum_{s_i=\pm 1} \exp(-\beta H(s, a.p.))}{\sum_{b.c.} \sum_{s_i=\pm 1} \exp(-\beta H(s, b.c.))\delta_{b.c.,a.p.}} = \frac{\langle \delta_{b.c.,a.p.} \rangle}{\langle \delta_{b.c.,p.} \rangle} . \hspace{1cm} (13)
\]

In the case of a surface with fixed position, the surface free energy is given by

\[
F_s = F_{a.p.} - F_{p.} = \ln Z_{p.} - \ln Z_{a.p.} = -\ln \frac{Z_{a.p.}}{Z_{p.}} , \hspace{1cm} (14)
\]

where \( F_{p.} \) and \( F_{a.p.} \) are the reduced free energies of the systems with periodic and antiperiodic boundary conditions, respectively. If we assume that there is no interface in the system with periodic boundary conditions and exactly one in the case of antiperiodic boundary conditions, we can take into account the entropy due to the free position of the interface in \( T \) direction by adding \( \ln T \),

\[
F_s = F_{a.p.} - F_{p.} + \ln T . \hspace{1cm} (15)
\]

We get a more appropriate description for finite systems if we take into account the occurrence of several interfaces, an even number for periodic and an odd number for antiperiodic boundary conditions. If we furthermore assume that these interfaces do not interact we get an improved expression

\[
\tanh(\exp(-F_{s,i} + \ln T)) = \frac{Z_{a.p.}}{Z_{p.}} \hspace{1cm} (16)
\]

for the surface free energy. If we resolve this equation with respect to \( F_{s,i} \) we get

\[
F_{s,i} = \ln T - \ln(\frac{1}{2}\ln(1 + \frac{Z_{a.p.}/Z_{p.}}{1 - Z_{a.p.}/Z_{p.}})). \hspace{1cm} (17)
\]
4 The Algorithm

I shall now describe an efficient algorithm to update the above explained system, where the type of boundary condition is a random variable. The simplest way to alter the boundary conditions is to propose a change of the coupling $J_{<ij>}$ of sites in the uppermost plane with sites in the lowermost plane from 1 to $-1$ or vice versa in a single Metropolis step. With high probability most of the spins $s_i$ and $s_j$ have the same sign in the case of periodic boundary conditions and different sign in the case of antiperiodic boundary conditions. Hence the acceptance rate of such a Metropolis step will be extremely small. This simple algorithm does not take into account that the physical interface can be built anywhere in the system and, what is even more important, that the interface wildly fluctuates close to the critical point.

The cluster algorithm is the natural candidate to find the physical surface structure. First one goes through the lattice and deletes the bonds with the standard probability \[ p_d = \exp(-\beta(1 + J_{<ij>} s_i s_j)). \] (18)

Then one searches for a sheet of deleted bonds that completely cuts the lattice in z-direction. If there is such a sheet the spins from the lowermost plane up to this sheet are flipped. This is a valid update, since the bonds in the sheet are deleted and the value of $J_{<ij>} s_i s_j$ for $i$ in the lowermost and $j$ in the uppermost plane is not changed when we alter the sign of $J_{<i,j>}$ and $s_i$.

In my simulations I alternate this boundary flip update with a standard single cluster update [21].

5 Numerical Results

I simulated the 3D Ising model on a simple cubic lattice with boundary conditions as dynamical variables at $\beta = 0.223, 0.224, 0.2255, 0.2275, 0.2327$ and 0.2391. For most of the simulations lattices of size $L \times L \times T$ with $T = 3L$ were used. In order to check for the $T$-dependence of the results at $\beta = 0.2275$ also simulations with $T = L/2, L, 2L$ were performed. The statistics of the simulations was 100000 times one single cluster update [21] plus one boundary flip update throughout. I measured the energy

\[ E = \sum_{<ij>} J_{<ij>} s_i s_j, \] (19)

the magnetization

\[ m = \frac{1}{L^2 \times T} \sum_i s_i \] (20)

and the type of boundary condition (b.c.) after each pair of single cluster plus boundary flip update. These data are used to calculate the energy
density of the system with periodic boundary conditions

\[ E_p = \frac{1}{L^2 \times T} \sum_{n=n_0}^{N} E \delta_{b.c.,p}, \]  

(21)

where \( n \) labels the measurements, and \( N \) is the number of measurements. The mean square magnetization of the system with periodic boundary conditions is

\[ \langle m^2 \rangle = \frac{\sum_{n=n_0}^{N} m^2 \delta_{b.c.,p}}{\sum_{n=n_0}^{N} \delta_{b.c.,p}}, \]  

(22)

and the surface energy density

\[ SE = \frac{1}{L^2} \left( \frac{\sum_{n=n_0}^{N} E \delta_{b.c.,p}}{\sum_{n=n_0}^{N} \delta_{b.c.,p}} - \frac{\sum_{n=n_0}^{N} E \delta_{b.c.,a.p.}}{\sum_{n=n_0}^{N} \delta_{b.c.,a.p.}} \right). \]  

(23)

The results for these quantities are summarized in table 1. For parameters where the fraction of configurations with antiperiodic boundary conditions is large the value for the surface energy is not reliable, since many of the configurations contain more than the minimal number of interfaces. A strong dependence of \( SE \) on \( L \) is visible.

Starting from the fraction of configurations with antiperiodic boundary conditions \( \langle \delta_{b.c.,a.p.} \rangle \) the reduced surface free energies \( F_s \) and \( F_{s,i} \) are determined following eqn. (15) and (17), respectively. The results are summarized in table 2. For \( F_s \geq 6 \) the difference between the two definitions \( F_s \) and \( F_{s,i} \) of the surface energy is smaller than the statistical errors. At \( \beta = 0.2275 \) I investigated the dependence of the surface free energy on \( T \). One can observe that \( F_{s,i} \) remains constant within errorbars for \( L = 10, 12 \) and 14 starting from \( T = L \). \( T = 3L \) seems to be safe not to spoil the results.

Using \( F_{s,i} \) I calculated the inverse correlation length of an 1D Ising model with \( 2\beta_{\text{eff}} = F_{s,i} \) following eq. (3). The results which are given in table 2 can be compared with the direct measurement of the mass of a 3D Ising model on a cylindrical lattice at \( \beta = 0.2275, 0.2327 \) and 0.2391 of ref. [2]. The numbers they give for \( E_0 \) in their table 1 are consistent with my results for the masses of the effective 1D Ising model within errorbars.

Similar to the surface energy the values of \( F_s/L^2 \) and \( F_{s,i}/L^2 \) which I give in table 2 displays a strong dependence on the lattice size. It seems difficult to extract the infinite \( L \) limit of the surface tension from these numbers. Motivated by free field theory (in ref. [3] we demonstrate that the long range properties of an interface in the rough phase of a 3D Ising model is well described by a massless free field theory), I tried to fit the surface free energy according to the Ansatz

\[ F_{s,i} = C + \sigma L^2. \]  

(24)

It turned out that the data fit very well to this Ansatz. The results of the fits are given in table 3.
Starting from the $\sigma$’s given in table 3 I did several fits to test the scaling law $\sigma = \sigma_0 t^\mu$. I used two different definitions for the reduced temperature, $t_1 = (\beta - \beta_c)/\beta_c$ and $t_2 = (T_c - T)/T_c$. In both cases I used $\beta_c = 0.221652$ given in ref. [10]. Remember that $t_1$ and $t_2$ are equivalent in the first order of a Taylor series around $T_c$. The results are given in table 4 and table 5. One can observe that it is necessary to go even closer to the critical temperature to overcome the ambiguity in the definition of the reduced temperature $t$. Taking into account this systematic errors I get as an estimate for the critical exponent $\mu = 1.24(3)$.

In order to get a better estimate for the critical amplitude of the surface tension $\sigma_0$ I used the results of ref. [10, 11] for $\nu$ combined with the scaling relation $\mu = 2\nu$ and determined

$$\sigma_0 = \sigma t^{-\mu}$$

from single measurements of $\sigma$. The results are given in table 6. Taking into account the uncertainty in the value of $\nu$ a final estimate $\sigma_0 = 1.5 \pm 0.1$ seems reasonable. Using the estimate $\xi_0^+ = 0.4783 \pm 0.0004$ of ref. [22] I get $R_+ = 0.34(2)$. Taking into account the deviation from the mean value of the results for the various binary alloys quoted in ref. [15] my result is well consistent with experiment and most of the recent Monte Carlo simulations [25, 2, 3, 7]. Since I have surface tensions for more $\beta$ values and $\beta$’s closer to the phase transition as the references quoted above I improved the control on finite $t$ effects. One should mention that earlier results of Monte Carlo simulation [23] and analytic calculations [24] were about 30% below the experimental value.

Let me finally comment on the performance of the algorithm. The autocorrelation times were of order 1 in units of the combined single cluster plus boundary flip update for all simulations quoted above. The simulation of the largest system ($36 \times 36 \times 108$) took 84h on an IBM risc station 6000. The drawback of the method is its limitation to small surface free energies. For $F_s > 9$ the fraction of configurations with antiperiodic boundary conditions becomes smaller than 1% and hence it is hard to get a sufficient statistic of configurations with antiperiodic boundary conditions. A solution of this problem might be found in a combination with multicanonical methods. But the most naive proposal of this kind, just to introduce a chemical potential that makes the antiperiodic boundary conditions more probable, fails. The flip from periodic boundary conditions to antiperiodic boundary conditions is allowed only if there is a sheet of deleted bonds in the system that cuts the lattice. The chemical potential just forces the system to stay longer with antiperiodic boundary conditions after such a flip. Hence the statistics of boundary flips is even reduced.

6 Conclusion

I presented an effective method to determine the surface tension of Ising systems. It should also be applicable to other discrete spin models. The
method allowed to obtain the surface tension very close \((T = 0.994 T_c)\) to the critical temperature with a high accuracy. The mass of the cylindrical 3D Ising system due to tunneling turned out to be given to a very good accuracy by the mass of an 1D Ising model with \(2\beta_{\text{eff}} = \text{surface free energy}\), which is consistent with the prediction of ref. \([18]\). But the finite size behavior of the surface free energy of the rough interface is well described by \(F_s = C + \sigma L^2\) leading to the prefactor predicted in ref. \([19]\).

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References

[1] H. Meyer-Ortmanns, T. Trappenberg, J. Stat. Phys. 58 (1990) 185;
    H. Meyer-Ortmanns, Proceedings of the XXIII. International Symposium
    on the Theory of Elementary Particles, ed.: E. Wieczorek, Ahrens
    shoop, GDR, 1989
[2] S. Klessinger, G. Münster, preprint Münster University, MS-TPI-92-13,
    May 1992, to be published in Nucl. Phys. B
[3] B.A. Berg, U. Hansmann, T. Neuhaus,
    preprint Florida State University FSU-SCRI-92-86, July 1992
[4] H. Gausterer, J. Potvin, C. Rebbi, S. Sanielevici, preprint Boston University,
    BU-HEP-92-16
[5] M. Hasenbusch, K. Pinn, preprint Münster University, MS-TPI-92-24,
    September 1992 in preparation
[6] K. Jansen, Y. Shen, San Diego preprint UCSD/PTH 92-02, BNL-45082,
    Jan. 1992
[7] M. Caselle, R. Fiore, F. Gliozzi, and S. Vinti, preprint Turin University,
    DFTT 23/92.
[8] B. Widom, J. Chem. Phys. 43 (1965) 3892
[9] B. Widom, in: Phase Transitions and Critical Phenomena, Vol.2, ed.:
    C. Domb, M. S. Green, Academic Press, London, 1971
[10] C.F. Baillie, R. Gupta, K.A. Hawick and G.S. Pawley Phys. Rev. B 45
    (1992) 10438
[11] J.-C. Le Guillou, J. Zinn-Justin, Phys. Rev. B \textbf{21} (1980) 3976; J. Zinn-Justin, in: Phase Transitions, Cargèse 1980, ed.: M. Lévy et al., Plenum Press, New York, 1982

[12] I. A. McLure, I. L. Pegg, J. Mol. Structure \textbf{80} (1982) 393

[13] H. L. Gielen, J. Thoen, O. B. Verbeke, J. Chem. Phys. \textbf{81} (1984) 6154

[14] M. R. Moldover, Phys. Rev. A \textbf{31} (1985) 1022

[15] H. Chaar, M. Moldover, J. Schmidt, J. Chem. Phys. \textbf{85} (1986) 418

[16] S. Fisk, B. Widom, J. Chem. Phys. \textbf{50} (1969) 3219

[17] D. Stauffer, M. Ferer, M. Wortis, Phys. Rev. Letters \textbf{29} (1972) 345

[18] C. Borgs, J. Z. Imbrie, Harvard preprint 91-0233

[19] G. Münster, Nucl. Phys. B \textbf{340} (1990) 559

[20] R. H. Swendsen, J.-S. Wang, Phys. Rev. Letters \textbf{58} (1987) 86

[21] U. Wolff, Phys. Rev. Letters \textbf{62} (1989) 361

[22] H. B. Tarko, M. E. Fisher, Phys. Rev. B \textbf{11} (1975) 1217

[23] K. Binder, Phys. Rev. A \textbf{25} (1982) 1699

[24] E. Brézin, S. Feng, Phys. Rev. B \textbf{29} (1984) 472

[25] K. K. Mon, Phys. Rev. Letters \textbf{60} (1988) 2749
Table 1: Data for 3-D Ising cylinders of size $L^2 \times T$ at $\beta = 0.223, 0.224, 0.2255, 0.2275, 0.2327$ and $0.2391$. $E_p$ denotes the energy density of the system with periodic boundary conditions, $< m^2 >$ is the expectation value of the square magnetization of the system with periodic boundary conditions. $ES$ is the difference of the energy with periodic and the energy with antiperiodic boundary conditions divided by the area $L^2$. $< \delta_{b.c.,a.p.} >$ gives the fraction of configurations with antiperiodic boundary conditions.

| $L$ | $T$ | $E_p$ | $< m^2 >$ | $ES$ | $< \delta_{b.c.,a.p.} >$ |
|-----|-----|-------|-----------|------|------------------|
| 4   | 12  | 0.5219(9) | 0.3586(14) | 1.364(41) | 0.4388(8) |
| 6   | 18  | 0.5435(5) | 0.4187(9)  | 2.607(40) | 0.2948(12) |
| 8   | 24  | 0.5524(3) | 0.4432(5)  | 3.247(41) | 0.1075(10) |
| 10  | 10  | 0.5541(4) | 0.4497(6)  | 3.378(57) | 0.0066(3)  |
| 10  | 30  | 0.5536(2) | 0.4460(3)  | 3.433(66) | 0.0192(5)  |
| 8   | 24  | 0.4861(4) | 0.3310(8)  | 2.498(42) | 0.2833(13) |
| 10  | 30  | 0.4905(3) | 0.3459(5)  | 2.986(44) | 0.1359(13) |
| 12  | 36  | 0.4917(2) | 0.3487(4)  | 3.166(55) | 0.0445(7)  |
| 14  | 42  | 0.4921(2) | 0.3493(3)  | 3.223(81) | 0.0100(3)  |
| 10  | 5   | 0.4219(8) | 0.2381(13) | 1.742(15) | 0.0782(11) |
| 10  | 10  | 0.4284(6) | 0.2518(10) | 2.167(24) | 0.1775(16) |
| 10  | 20  | 0.4250(5) | 0.2334(9)  | 2.021(39) | 0.2908(15) |
| 10  | 30  | 0.4231(4) | 0.2176(9)  | 1.810(50) | 0.3633(13) |
| 12  | 6   | 0.4227(7) | 0.2325(12) | 1.877(17) | 0.0551(10) |
| 12  | 12  | 0.4288(5) | 0.2472(9)  | 2.383(29) | 0.1179(16) |
| 12  | 24  | 0.4272(4) | 0.2377(7)  | 2.360(39) | 0.2061(17) |
| 12  | 36  | 0.4268(3) | 0.2301(7)  | 2.269(49) | 0.2741(16) |
| 14  | 14  | 0.4296(4) | 0.2461(8)  | 2.604(30) | 0.0683(13) |
| 14  | 28  | 0.4294(3) | 0.2415(6)  | 2.590(40) | 0.1232(15) |
| 14  | 42  | 0.4293(3) | 0.2388(5)  | 2.605(47) | 0.1698(16) |
| 16  | 48  | 0.4301(2) | 0.2418(4)  | 2.706(48) | 0.0860(12) |
| 18  | 54  | 0.4302(2) | 0.2422(3)  | 2.836(62) | 0.0378(8)  |
\[
\begin{array}{cccccc}
L & T & E_p & \langle m^2 \rangle & ES & \langle \delta_{b,c,a,p} \rangle \\
\beta=0.2255 & & & & & \\
14 & 42 & 0.3982(3) & 0.1734(7) & 1.805(53) & 0.3281(16) \\
16 & 48 & 0.4001(3) & 0.1808(6) & 2.121(51) & 0.2540(18) \\
18 & 54 & 0.4012(2) & 0.1852(5) & 2.310(46) & 0.1752(16) \\
20 & 60 & 0.4018(2) & 0.1872(4) & 2.426(47) & 0.1076(14) \\
24 & 72 & 0.4022(1) & 0.1885(3) & 2.490(68) & 0.0284(7) \\
\beta=0.224 & & & & & \\
14 & 42 & 0.3731(3) & 0.1167(8) & 1.014(56) & 0.4252(12) \\
18 & 54 & 0.3750(3) & 0.1247(7) & 1.467(56) & 0.3553(17) \\
24 & 72 & 0.3778(2) & 0.1362(4) & 1.982(50) & 0.1884(20) \\
30 & 90 & 0.3788(1) & 0.1395(3) & 2.312(65) & 0.0575(12) \\
\beta=0.223 & & & & & \\
8 & 24 & 0.3648(5) & 0.1077(9) & 0.380(52) & 0.4821(5) \\
12 & 36 & 0.3588(4) & 0.0879(8) & 0.469(58) & 0.4720(6) \\
18 & 54 & 0.3572(3) & 0.0812(8) & 0.744(72) & 0.4423(13) \\
24 & 72 & 0.3586(2) & 0.0867(6) & 1.186(59) & 0.3754(19) \\
30 & 90 & 0.3600(2) & 0.0938(4) & 1.605(58) & 0.2677(23) \\
36 & 108 & 0.3608(1) & 0.0975(3) & 1.845(56) & 0.1437(21) \\
\end{array}
\]
Table 2: Results for the surface tension and the mass ($mass_{1d}$) of an effective Ising model with $2\beta_{\text{eff}} = F_{s,i}$ are given. $F_s$ and $F_{s,i}$ are explained in the text.

| $L$ | $T$ | $F_s$    | $F_s/L^2$ | $F_{s,i}$  | $F_{s,i}/L^2$ | $mass_{1d}$ |
|-----|-----|----------|-----------|------------|---------------|-------------|
|     |     |          |           |            |               |             |
| 4   | 12  | 2.731(3) | 0.1707(2) | 2.436(6)   | 0.1523(4)     | 0.1755(10)  |
| 6   | 18  | 3.763(6) | 0.1045(2) | 3.699(7)   | 0.1028(2)     | 0.0495(3)   |
| 8   | 24  | 5.294(11)| 0.0827(2) | 5.289(11)  | 0.0827(2)     | 0.01010(11) |
| 10  | 10  | 7.311(40)| 0.0731(4) | 7.311(40)  | 0.0731(4)     | 0.00134(5)  |
| 10  | 30  | 7.335(24)| 0.0734(3) | 7.335(24)  | 0.0734(3)     | 0.00130(3)  |
|     |     |          |           |            |               |             |
| 8   | 24  | 4.106(7) | 0.06416(10)| 4.050(7)   | 0.06328(12)   | 0.0348(2)   |
| 10  | 30  | 5.251(11)| 0.05251(11)| 5.243(11)  | 0.05243(11)   | 0.01057(12) |
| 12  | 36  | 6.649(17)| 0.04618(12)| 6.649(17)  | 0.04617(12)   | 0.00259(4)  |
| 14  | 42  | 8.330(33)| 0.04250(17)| 8.330(33)  | 0.04250(17)   | 0.00048(2)  |
|     |     |          |           |            |               |             |
| 10  | 5   | 4.076(15)| 0.04076(15)| 4.074(15)  | 0.04074(15)   | 0.0340(5)   |
| 10  | 10  | 3.836(11)| 0.03836(11)| 3.820(11)  | 0.03820(11)   | 0.0439(5)   |
| 10  | 20  | 3.887(7) | 0.03887(7) | 3.827(8)   | 0.03827(8)    | 0.0436(4)   |
| 10  | 30  | 3.962(6) | 0.03962(6) | 3.834(8)   | 0.03834(7)    | 0.0433(4)   |
|     |     |          |           |            |               |             |
| 12  | 6   | 4.634(19)| 0.03218(13)| 4.633(19)  | 0.03217(13)   | 0.0195(4)   |
| 12  | 12  | 4.497(15)| 0.03123(10)| 4.491(15)  | 0.03119(10)   | 0.0224(3)   |
| 12  | 24  | 4.527(10)| 0.03144(7) | 4.504(11)  | 0.03128(7)    | 0.0221(2)   |
| 12  | 36  | 4.557(8) | 0.03165(6) | 4.507(9)   | 0.03130(6)    | 0.0221(2)   |
|     |     |          |           |            |               |             |
| 14  | 14  | 5.252(20)| 0.02679(10)| 5.250(20)  | 0.02679(10)   | 0.0105(2)   |
| 14  | 28  | 5.294(13)| 0.02701(7) | 5.288(14)  | 0.02698(7)    | 0.01010(14) |
| 14  | 42  | 5.325(11)| 0.02717(6) | 5.311(11)  | 0.02710(6)    | 0.00987(11) |
| 16  | 48  | 6.234(15)| 0.02435(6) | 6.231(15)  | 0.02434(6)    | 0.00393(6)  |
| 18  | 54  | 7.225(21)| 0.02230(6) | 7.225(21)  | 0.02230(6)    | 0.00146(3)  |
Table 3: Results of fits of the form $F_{s,i} = C + \sigma L^2$ are given. Only values from the largest $T$ are included in the fits. $\chi^2$/d.o.f. denotes the square deviation per degrees of freedom.

| $\beta$ | $L$'s used | $C$ | $\sigma$ | $\chi^2$/d.o.f. |
|---------|------------|-----|---------|-----------------|
| 0.2391  | 6,8,10     | 1.65(2) | 0.0568(3) | 0.002           |
| 0.2327  | 8,10,12,14 | 1.97(2) | 0.0325(2) | 1.74            |
| 0.2275  | 12,14,16,18| 2.32(2) | 0.01521(11)| 1.69           |
| 0.2255  | 14,16,18,20,24| 2.59(2) | 0.00904(6) | 0.08           |
| 0.224   | 18,24,30   | 2.87(2) | 0.00492(4) | 0.63           |
| 0.223   | 24,30,36   | 3.19(2) | 0.00252(3) | 0.002          |
Table 4: Fits of the form $\sigma = \sigma_0 t_1^\mu$, where $t_1 = (\beta - \beta_c)/\beta_c$. The labels 1, 2, 3, 4, 5 and 6 correspond to $\beta = 0.2391, 0.2327, 0.2275, 0.2255, 0.224$ and 0.223, respectively.

| input    | $\mu$   | $\sigma_0$ | $\chi^2$/d.o.f. |
|----------|---------|------------|-----------------|
| 1,2,3,4,5,6 | 1.217(4) | 1.25(2)    | 0.89            |
| 2,3,4,5,6  | 1.218(5) | 1.26(3)    | 1.15            |
| 3,4,5,6    | 1.228(8) | 1.32(4)    | 0.58            |
| 4,5,6      | 1.220(12)| 1.27(7)    | 0.42            |
| 1,2,3,4,5  | 1.217(4) | 1.25(2)    | 0.89            |
| 2,3,4,5    | 1.218(6) | 1.26(3)    | 1.15            |
| 3,4,5      | 1.237(12)| 1.36(7)    | 0.09            |

Table 5: Fits of the form $\sigma = \sigma_0 t_2^\mu$, where $t_2 = (T_c - T)/T_c$. The labels 1, 2, 3, 4, 5 and 6 correspond to $\beta = 0.2391, 0.2327, 0.2275, 0.2255, 0.224$ and 0.223, respectively.

| input    | $\mu$   | $\sigma_0$ | $\chi^2$/d.o.f. |
|----------|---------|------------|-----------------|
| 1,2,3,4,5,6 | 1.256(4) | 1.51(2)    | 2.5             |
| 2,3,4,5,6  | 1.246(5) | 1.45(3)    | 0.8             |
| 3,4,5,6    | 1.246(9) | 1.45(5)    | 1.2             |
| 4,5,6      | 1.234(13)| 1.37(8)    | 0.7             |
| 1,2,3,4,5  | 1.260(4) | 1.53(2)    | 1.6             |
| 2,3,4,5    | 1.250(6) | 1.47(3)    | 0.4             |
| 3,4,5      | 1.258(12)| 1.52(8)    | 0.3             |
Table 6: Results for $\sigma_0 = \sigma t_1^{-\mu}$ and $\sigma_0 = \sigma t_1^{1-\mu}$ using the value of single measurements for $\sigma$ and given $\mu = 1.248$ and 1.26.

| $\beta$ | $\sigma_0, t_1$ | $\sigma_0, t_2$ |
|---------|----------------|----------------|
| $\mu = 1.248$ |                |                |
| 0.2391  | 1.355(7)       | 1.490(8)       |
| 0.2327  | 1.372(8)       | 1.458(9)       |
| 0.2275  | 1.420(10)      | 1.467(11)      |
| 0.2255  | 1.423(9)       | 1.454(10)      |
| 0.2240  | 1.435(12)      | 1.454(12)      |
| 0.2230  | 1.469(18)      | 1.480(18)      |
| $\mu = 1.26$ |                |                |
| 0.2391  | 1.397(7)       | 1.537(8)       |
| 0.2327  | 1.422(9)       | 1.512(9)       |
| 0.2275  | 1.483(11)      | 1.533(11)      |
| 0.2255  | 1.494(10)      | 1.527(10)      |
| 0.2240  | 1.515(12)      | 1.535(13)      |
| 0.2230  | 1.562(19)      | 1.574(19)      |