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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 [1-6], while in reference [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 $\sigma = \tau\beta$, where τ is the surface tension and $\beta = \frac{1}{k_b T}$ the inverse temperature, vanishes according to the scaling law

$$\sigma = \sigma_0 t^{\mu} , \tag{1}$$

where $t = (T_c - T)/T_c$, and σ_0 is the critical amplitude of the reduced interface tension. Widom's scaling law [8, 9]

$$\mu = (D - 1)\,\nu \tag{2}$$

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relates the universal critical exponent μ to the critical exponent of the correlation length

$$\xi = \xi_0 t^{-\nu} \tag{3}$$

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 ε-expansion predicts $\nu = 0.630(2)$ [11]. The experimental [12-15] value for μ is $\mu = 1.26(1)$, consistent with Widom's 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

$$R_+ = \sigma_0 (\xi_0^+)^2 = 0.386 \tag{4}$$

[15], where ξ_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

$$\xi_L = \frac{1}{2} \exp(\sigma L^2) . \tag{5}$$

A semiclassical instantion calculation [19] however predicts

$$\xi_L = c \exp(\sigma L^2) , \tag{6}$$

where c depends on the temperature and is not equal to 1/2.

In order to understand this discrepancy I compared the correlation length of an 1D Ising model with a coupling β_{eff} given by

$$2 \beta_{\text{eff}} = F_s , \tag{7}$$

which is exact for a 1^3 Ising system, and where F_s is the reduced surface free energy of the 3D system, with the correlation length measured in reference [2] for 3D Ising cylinders.

The correlation length ξ of a 1D Ising model is given by

$$\xi = \frac{1}{\ln ((1 + v)/(1 - v))} , \tag{8}$$

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

$$\xi = \frac{1}{2v} \tag{9}$$

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

$$H(s, \mathrm{bc}) = - \sum_{\langle ij \rangle} J_{\langle ij \rangle} s_i s_j . \tag{10}$$

When periodic (p) boundary conditions (bc) are employed, then $J_{\langle ij \rangle} = 1$ for all nearest neighbor pairs. When antiperiodic (ap) boundary conditions are employed, then $J_{\langle ij \rangle} = -1$ for bonds $\langle ij \rangle$ connecting the lowermost and uppermost plane of the lattice, while all other nearest neighbor pairs keep $J_{\langle ij \rangle} = 1$.

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

$$Z = \sum_{\mathrm{bc}} \sum_{s_i = \pm 1} \exp(- \beta H(s, \mathrm{bc})) . \tag{11}$$

The fraction of configurations with antiperiodic boundary conditions is given by the ratio Z_{ap}/Z,

$$\begin{aligned} \frac{Z_{\mathrm{ap}}}{Z} &= \frac{\sum_{s_i = \pm 1} \exp(- \beta H(s, \mathrm{ap}))}{Z} \\ &= \frac{\sum_{\mathrm{bc}} \sum_{s_i = \pm 1} \exp(- \beta H(s, \mathrm{bc}))\, \delta_{\mathrm{bc, ap}}}{Z} \\ &= \langle \delta_{\mathrm{bc, ap}} \rangle . \end{aligned} \tag{12}$$

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

$$\frac{Z_{\mathrm{ap}}}{Z_{\mathrm{p}}} = \frac{\frac{Z_{\mathrm{ap}}}{Z}}{\frac{Z_{\mathrm{p}}}{Z}} = \frac{\langle \delta_{\mathrm{bc, ap}} \rangle}{\delta_{\mathrm{bc, p}}} \tag{13}$$

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

$$F_{\mathrm{s}} = F_{\mathrm{ap}} - F_{\mathrm{p}} = \ln Z_{\mathrm{p}} - \ln Z_{\mathrm{ap}} = - \ln \frac{Z_{\mathrm{ap}}}{Z_{\mathrm{p}}} , \tag{14}$$

where F_{p} and F_{ap} 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 $\ln T$,

$$F_s = F_{ap} - F_p + \ln T \,. \tag{15}$$

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

$$\tanh\,(\exp(-F_{s,\,i} + \ln T)) = \frac{Z_{ap}}{Z_p} \tag{16}$$

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

$$F_{s,\,i} = \ln T - \ln\left(\frac{1}{2}\ln\left(\frac{1 + Z_{ap}/Z_p}{1 - Z_{ap}/Z_p}\right)\right) . \tag{17}$$

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 $J_{\langle ij\rangle}$ 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 signs 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 the fact 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 method to compute the interface free energy proposed in reference [20], where one has to measure the exponential of the product of the magnetisation of neighboring layers of the system with periodic boundary conditions, is closely related to such an update. Here one recovers the problems as a very large variance of the observable. The authors of reference [20] tried to overcome this drawback by introducing a number of Hamiltonians, which interpolate between periodic and antiperiodic boundary conditions.

These problems can be resolved directly by using a cluster algorithm. Let us first consider fixed boundary conditions where the spins at the bottom and the top layer of the lattice are fixed to plus one $(+\,+\,)$ or the spins at the bottom layer are fixed to plus one while spins at the top layer are fixed to minus one $(+\,-\,)$. To update a system that contains $(+\,+\,)$ and $(+\,-\,)$ boundary conditions as random variables one can use a standard cluster algorithm [21, 22]. One has to freeze all the bonds within the top and bottom layer of the lattice to keep all spins parallel within these layers. All other bonds are deleted with the standard probability [21, 22]

$$p_d = \exp(-\beta\,(1 + s_i\,s_j)) \tag{18}$$

or frozen else. In the case of the Swendsen-Wang algorithm one now flips all clusters with probability 1/2, only the cluster that contains the bottom layer keeps its sign. (If we allow also for $(-\,-\,)$ and $(-\,+\,)$ boundary conditions we can skip this modification.) This means that, if the bottom and top layer belong to different clusters, one switches from one type of the boundary conditions to the other with probability 1/2. One should mention that, if we start with

(+ −) boundary conditions the two boundary layers will always belong to two different clusters, since the clusters of a standard cluster algorithm [21, 22] contain only spins of one sign. The single cluster algorithm can also be used without any modification.

In order to handle with (ap) and (p) boundary conditions some modifications are needed. First one has to give the delete probability also for a negative coupling $J_{\langle ij\rangle} = -1$

$$p_d = \exp(-\beta (1 + J_{\langle ij\rangle} s_i s_j)) . \tag{19}$$

After deleting or freezing the bonds of the system one searches for a sheet of deleted bonds that completely cuts the lattice in z-direction. If there is such a sheet, the spins between the bottom of the system and this sheet and the sign of the coupling $J_{\langle ij\rangle}$ connecting top and bottom are flipped. This is a valid update, since the bonds in the sheet are deleted and the value of $J_{\langle ij\rangle} s_i s_j$ for i in the lowermost and j in the uppermost plane is not changed when we alter the sign of $J_{\langle i,j\rangle}$ and s_i.

For those who actually want to implement this update : you have to construct all clusters that contain sites of the lowermost layer of the system. The easiest way to do this is to start growing clusters in this layer as long as there are sites which are not contained in a cluster. In order to get a notion of what is the part of the cluster below the boundary and above the boundary, introduce an auxiliary variable $p(i)$ which can either take the value 1 or − 1 depending on the lattice site i. When you start the cluster at the lattice site i_0 set $p(i_0) = 1$. When you grow the cluster, a new site i get its $p(i)$ from the site j which is already in the cluster and where it is frozen to. When the corresponding bond $\langle ij\rangle$ connects bottom and top we set $p(i) = -p(j)$ and else $p(i) = p(j)$. If now two sites which are already taken into the cluster are frozen together and have an unconsistent p the cluster wraps around the lattice and the boundary condition update is forbidden. When this is not the case for any of the clusters we can flip the boundary conditions when we flip the spins of either the upper or lower part of all the clusters that contain sites at the bottom layer.

In my simulations I alternate this boundary flip update with a standard single cluster update [22].

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 were 100 000 times one single cluster update [22] plus one boundary flip update throughout. I measured the energy

$$E = \sum_{\langle ij\rangle} J_{\langle ij\rangle} s_i s_j , \tag{20}$$

the magnetization

$$m = \frac{1}{L^2 \times T} \sum_i s_i \tag{21}$$

and the type of boundary condition (bc) 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

$$E_p = \frac{1}{L^2 \times T} \frac{\sum_{n=n_0}^{N} E\delta_{bc,\,p}}{\sum_{n=n_0}^{N} \delta_{bc,\,p}}, \tag{22}$$

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

$$\langle m^2 \rangle = \frac{\sum_{n=n_0}^{N} m^2\,\delta_{bc,\,p}}{\sum_{n=n_0}^{N} \delta_{bc,\,p}}, \tag{23}$$

and the surface energy density

$$E_s = \frac{1}{L^2}\left(\frac{\sum_{n=n_0}^{N} E\delta_{bc,\,p}}{\sum_{n=n_0}^{N} \delta_{bc,\,p}} - \frac{\sum_{n=n_0}^{N} E\delta_{bc,\,ap}}{\sum_{n=n_0}^{N} \delta_{bc,\,ap}} \right). \tag{24}$$

The results for these quantities are summarized in table I. 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 E_s, on L is visible.

Table I. — *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,* $\langle m^2 \rangle$ *is the expectation value of the square magnetization of the system with periodic boundary conditions.* E_s *is the difference of the energy with periodic and the energy with antiperiodic boundary conditions divided by the area* L^2. $\langle \delta_{b.c.,\,a.p.} \rangle$ *gives the fraction of configurations with antiperiodic boundary conditions.*

L	T	E_p	$< m^2 >$	E_s	$< \delta_{b.c.,a.p.} >$
β=0.2391					
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)
β=0.2327					
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)

Table I (*continued*).

β=0.2275					
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)
β=0.2255					
14	42	0.3982(3)	0.1734(7)	1.805(53)	.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)
β=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)
β=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)

Starting from the fraction of configuration with antiperiodic boundary conditions $\langle \delta_{bc,\,ap} \rangle$ the reduced surface free energies F_s and $F_{s,\,1}$ are determined following equation (15) and (17), respectively. The results are summarized in table II. For $F_s \geq 6$ the difference between the two definitions F_s and $F_{s,\,1}$ 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

Table II. — *Results for the surface tension and the inverse of the correlation length* ξ_{1d}^{-1} *of an effective Ising model with* $2\,\beta_{eff} = F_{s,\,1}$ *are given.* F_s *and* $F_{s,\,1}$ *are explained in the text.*

L	T	F_s	F_s/L^2	$F_{s,s}$	$F_{s,s}/L^2$	ξ_{1d}^{-1}
β=0.2391						
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)
β=0.2327						
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)
β=0.2275						
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 II (*continued*).

β=0.2255						
14	42	4.455(7)	0.02273(4)	4.365(9)	0.02227(5)	0.0254(2)
16	48	4.949(9)	0.01933(4)	4.908(10)	0.01917(4)	0.0148(1)
18	54	5.537(11)	0.01709(4)	5.522(11)	0.01704(4)	0.00800(9)
20	60	6.210(15)	0.01552(4)	6.205(15)	0.01551(4)	0.00404(6)
24	72	7.808(25)	0.01356(4)	7.807(25)	0.01355(4)	0.00081(2)
β=0.224						
14	42	4.039(5)	0.02061(2)	3.789(8)	0.01933(4)	0.0452(3)
18	54	4.585(7)	0.01415(2)	4.467(9)	0.01379(3)	0.0230(2)
24	72	5.737(13)	0.00996(2)	5.719(13)	0.00993(2)	0.00657(8)
30	90	7.298(22)	0.00811(2)	7.296(22)	0.00811(2)	0.00136(3)
β=0.223						
8	24	3.250(2)	0.05078(3)	2.669(9)	0.04170(13)	0.139(1)
12	36	3.696(3)	0.02566(2)	3.218(8)	0.02235(6)	0.0801(6)
18	54	4.221(6)	.01303(2)	3.912(11)	0.01207(3)	0.0400(4)
24	72	4.786(8)	0.00831(1)	4.641(11)	0.00806(2)	0.0193(2)
30	90	5.506(12)	0.00612(1)	5.459(13)	0.00607(1)	0.00852(10)
36	108	6.467(17)	0.00500(1)	6.457(17)	0.00498(1)	0.00314(5)

observe that $F_{s,1}$ remains constant within error bars 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 a 1D Ising model with $2\beta_{\text{eff}} = F_{s,i}$ following equation (8). The results which are given in table II 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 reference [2]. The numbers they give for E_{0a} in their table I are consistent with my results for the inverse correlation length of the effective 1D Ising model within error bars.

Similar to the surface energy the values of F_s/L^2 and $F_{s,1}/L^2$ which I give in table II display 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. [5] we demonstrate that the long range properties of an interface in the rough phase of a 3D Ising model are well described by a massless free field theory), I tried to fit the reduced surface free energy according to the Ansatz

$$F_{s,1} = C + \sigma L^2 \tag{25}$$

It turned out that the data fit very well to this Ansatz. The results of the fits are given in table III.

Table III. — *Results of fits of the form* $F_{s,1} = C + \sigma L^2$ *are given. Only values from the largest T are included in the fits.* χ^2/d.o.f. *denotes the square deviation per degrees of freedom.*

β	L's used	C	σ	χ^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

Starting from the σ s given in table III 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 reference [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 IV and table V. 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 $\mu = 1.24$ (3) as an estimate for the critical exponent.

In order to get a better estimate for the critical amplitude of the surface tension σ_0 I used the results of references [10, 11] for ν combined with the scaling relation $\mu = 2\,\nu$ and determined

$$\sigma_0 = \sigma t^{-\mu} \tag{26}$$

from single measurements of σ. The results are given in table VI. Taking into account the uncertainty in the value of ν a final estimate $\sigma_0 = 1.5 \pm 0.1$ seems to be reasonable. Using the estimate $\xi_0^+ = 0.4783 \pm 0.0004$ of reference [23] 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 reference [15] my result is well consistent with experiments and most of the recent Monte Carlo

Table IV. — *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	μ	σ_0	χ^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 V. — *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	μ	σ_0	χ^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 VI. — *Results of* $\sigma_0 = \sigma t_1^{-\mu}$ *and* $\sigma_0 = \sigma t_2^{-\mu}$ *using the value of single measurements for* σ *and given* $\mu = 1.248$ *and* 1.26.

β	σ_0, t_1	σ_0, t_2
μ=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)
μ=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)

simulations [26, 2, 3, 7]. Since I have surface tensions for more β values and β'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 simulations [24] and analytic calculations [25] 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 84 h 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 are 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 correlation length of the cylindrical 3D Ising system in the low temperature phase turned out to be given to a very good accuracy by the mass of a 1D Ising model with $2\,\beta_{\text{eff}}$ = reduced surface free energy, which is consistent with the prediction of ref. [18]. But the finite size behavior of the reduced surface free energy of the rough interface is well described by $F_s = C + \sigma L^2$ leading to the prefactor predicted in reference [19].

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