Surface Tension, Surface Stiffness, and Surface Width of the 3-dimensional Ising Model on a Cubic Lattice

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We compute properties of the interface of the 3-dimensional Ising model for a wide range of temperatures and for interface extensions up to 64 by 64. The interface tension is obtained by integrating the surface energy density over the inverse temperature. The surface stiffness coefficient is determined. We also study universal quantities like ^{2} and ^{2}. The behavior of the interfacial width on lattices up to $512 \times 512 \times 27$ is also investigated.

Here we present a numerical study of 3-d Ising interfacial properties with focus on the precise determination of interface tension and interface stiffness over a wide range of temperatures. A detailed exposition of our work can be found in [1].

1. THE MODEL

We consider a simple cubic lattice with extension L in x– and y-direction and with extension $T = 2D + 1$ in z-direction. The lattice sites $i = (i_x; i_y; i_z)$ have integer coordinates, and the z-coordinate runs from $-D$ to $+D$. The Ising model is defined by the partition function

$$Z = \sum_{\{\sigma_i = \pm 1\}} \exp(-H); \qquad (1)$$

where

$$H = -\sum_{<i;j>} k_{ij} \sigma_i \sigma_j: \qquad (2)$$

The lattice becomes a torus by imposing geometrical periodic boundary conditions in all three directions. For the Ising spins σ_i we will use two different boundary conditions: Periodic boundary conditions are defined by letting $k_{ij} = 1$ for all links $<i;j>$. To define antiperiodic boundary

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talk presented by K. Pinn

conditions in z-direction, we also set $k_{ij} = 1$ with the exception of the links connecting the uppermost plane ($z = +D$) with the lowermost plane ($z = -D$). These links carry an antiferromagnetic factor $k_{ij} = -1$.

2. INTERFACIAL PROPERTIES

We adopt the following definition of the interfacial width: A magnetization profile for lattice planes perpendicular to the z-direction is defined by $M(i_z) = L^{-2} \sum_{i_x;i_y} \sigma_i$. The antiperiodic boundary condition allows us to shift the configuration in z-direction such that the interface comes close to $i_z = 0$. We introduce an auxiliary coordinate z that assumes half-integer values (labelling positions between adjacent lattice layers perpendicular to the z-direction). Following [2], a normalized magnetization gradient is defined as

$$\rho(z) = \frac{M(z + \frac{1}{2}) - M(z - \frac{1}{2})}{M(D) - M(-D)}: \qquad (3)$$

For a given spin configuration, the position of the interface is defined as $\sum \rho(z) z$. The square of the interface width is then defined [3,2] as

$$W^2 = \sum_z \rho(z) z^2 - \left(\sum_z \rho(z) z \right)^2: \qquad (4)$$

Especially on small lattices, fluctuations in the two bulk phases can deteriorate the results. Due

to bubbles, $\rho(z)$ can be accidentally large even far away from the interface position. We therefore also consider the interface width measured on the configurations after a removal of all bubbles.

We now turn to the definition of the interface tension. Let us assume that there is exactly one interface in the system with antiperiodic boundary conditions, and that there are no interfaces in the periodic system. Then the interfacial free energy is $F_s = F_{a.p.} - F_{p.} + \ln T$, where $F_{a.p.}$ ($F_{p.}$) is the free energy ($= -\ln Z$) of the system with antiperiodic (periodic) boundary in z-direction. For a discussion of the case of several interfaces see [1]. The interface tension is defined as the limit $\sigma = \lim_{L \to \infty} F_s / L^2$.

In general one has no direct access to the partition function in Monte Carlo simulations, except for not too large systems, cf. [4]. Note, however, that

$$\frac{\partial F_s}{\partial \beta} = \langle H \rangle_{i,a.p.} - \langle H \rangle_{i,p.} \equiv E_s . \qquad (5)$$

By integration one obtains

$$F_s(\beta) = F_s(\beta_0) + \int_{\beta_0}^{\beta} d\beta' E_s(\beta') ; \qquad (6)$$

where β_0 is arbitrary. Our approach is to compute by Monte Carlo simulation the surface energy for β-values ranging from the critical region around β_c ($= 0.221652(3)$ [5]) up to $\beta_0 \approx 0.6$. For large β we can employ a low temperature expansion by Weeks et al. (published in an article by Shaw and Fisher [6]) to obtain $F_s(\beta_0)$. Note that it is also possible to start the integration at small β [1]. (To the best of our knowledge, the integration method to obtain surface free energies was first used by Bürkner and Stauffer [7]).

In the theory of rough interfaces the surface stiffness coefficient κ plays an important role. If by suitably chosen boundary conditions the low temperature interface is forced to make an angle θ with e.g. the x-axis, one defines (see e.g. [8]),

$$\kappa = \sigma(0) + \frac{d^2 \sigma}{d\theta^2} \bigg|_{\theta = 0} . \qquad (7)$$

Capillary wave theory says that the long distance properties of the interface should by encoded in a 2-dimensional Gaussian model with Hamiltonian

$$H_0 = \frac{1}{2} \kappa_e \sum_{<i,j>} (h_i - h_j)^2 ; \qquad (8)$$

and $\kappa_e = 1/\sigma$. Long distance properties are most systematically studied via the block spin renormalization group. For the Gaussian model defined through eq. (8) one defines block spins ψ_I as averages over cubic blocks I of size L_B^2, i.e., $\psi_I = L_B^{-2} \sum_{i \in I} h_i$. We define the quantities

$$A_{i;l}^{(0)} = h \frac{1}{l^2} \sum_{(I,J)} (\psi_I - \psi_J)^2 i ; \qquad (9)$$

where I and J are nearest neighbors in the block lattice for $i = 1$, and next-to-nearest neighbors for $i = 2$. l is the extension of the block lattice, i.e. $l = L/L_B$. For the Gaussian model, the A's can be computed exactly. For the Ising model, block spin "height variables" h_I are defined as follows: The blocks I are sets that are quadratic in $x - y$ direction with extension $L_B \times L_B$ and that extend through the whole lattice in z-direction. For every block, a magnetization profile and an interface position can be determined exactly as in the case of the full lattice. We define $h_I =$ interface position in block I. Note that the blocked height variables can also be defined "with and without bubbles". Blocked observables for the Ising interface are introduced analogously to eq. (9), and are denoted by $A_{i;l}^{(Ising)}$. For a rough Ising interface, we define an effective coupling κ_e as follows:

$$\kappa_e = \lim_{L_B \to \infty} \frac{A_{i;l}^{(Ising)}}{A_{i;l}^{(0)}} . \qquad (10)$$

Of course, we expect that the so defined κ_e does not depend on i or l.

3. MONTE CARLO RESULTS

We did simulations with antiperiodic boundary conditions in z-direction on lattices with $L = 8, 16, 32, 64$ for β-values ranging from the bulk critical region up to $\beta = 0.6$. For many β-values we made runs with different D to control the effects of a finite thickness of the lattice. In total, we made more than 250 different simulations with

antiperiodic boundary conditions. Typically, we made 10000 measurements of several quantities, separated always by 8 cluster updates with the Hasenbusch-Meyer cluster algorithm for Ising interfaces [9]. The simulations supplied us with a sufficiently dense grid of -values for the energies $E_{a;p}$.

For most of the -values, we fortunately did not have to do extra simulations to access the energies with periodic boundary E_p. Instead we used the diagonal Pade approximation of the low temperature series by Bhanot et al. [10]. For smaller -values we used the cluster Monte Carlo method to determine E_p.

In order to do the integration over we interpolated the data with cubic splines. The integration was then started at $= 0:6$, where the integration constant can be safely taken from the low temperature series.

Already for moderate surface extension L, the surface free energy was found to behave with very good precision like $F_s = C_s + {}^0 L^2$. It was therefore natural to identify the coefficient ^{0} with the surface tension .

The results for the free energies for $L = 8$, 16, 32 and 64 were then used to make fits with $F_s = C_s + L^2$ in order to obtain estimates for the surface tension . In table 1 we display a few of our results. Our results show a significant deviation from a prediction by Shaw and Fisher [6] based on an analysis of the low temperature series. A detailed comparison will be published elsewhere [13].

We fitted our results for to the critical law $= {}_0 t$, using both of the two definitions $t = 1 {}_c=$ and $t = =_c 1$. We also varied the interval over which the -dependence of was fitted. The fits were always done using four different -values. The results based on the two different definitions of t were statistically incompatible, showing that one is still not close enough to criticality. However, taking systematic effects into account, we consider our results consistent with $1:26$. The results for the critical amplitude $_0$ show even stronger dependency on the type of the fit, and we can not say very much more than that ln $_0$ is probably something between $0:2$ and $0:4$.

In order to study the behavior of the product ^{2} we tried to determine the correlation length from the simulations of the system with periodic boundary conditions. We defined via the decay of the connected 2-point correlation function of the absolute value of the time-slice magnetization. Our results are nicely consistent with low temperature series [11].

We measured the block spin correlation functions $A_{i;1}^{(Ising)}$ and studied the quantities ${}_e^{i;1}( ) = A_{i;1}^{(Ising)}(L_B =)=A_{i;1}^{(0)}(L_B = 1)$ (measured on the configurations with the bubbles removed). The values for the different i;1 and 's turned out to be fairly consistent within the statistical accuracy. Our estimates for $_e$ were then determined by averaging over ${}_e^{i;1}$ with $i = 1$ and $i = 2$. Some of our results are shown in table 1.

In figure 1, we show our results for two combined quantities, namely ^{2} and ^{2}. In the product ^{2}, the exponents and 2 of the reduced temperature t should cancel, and we expect that this product should be fairly constant in a neighborhood of the critical point. The full line in the figure was obtained by combining our ^{0}s from the integration method with the correlation lengths as obtained from the Pade.

Since we do not know the error of the Pade approximation of the low temperature series we base our error estimate for this quantity on our error bars for the measured correlation length and on the statistical errors on the surface tension . We estimate the relative precision of our results for ^{2} to be around 5 per cent for the smaller 's, certainly better in the large region. This takes into account statistical errors only. There might also be systematic errors (due to too small L's) in the surface tension close to the critical point. They might be responsible for another 5 percent relative uncertainty. The points with error bars in the figure show the product ^{2}. The plot shows that in the critical limit the surface stiffness becomes the same as the interface tension. This is a consequence of the restoration of rotational symmetry at the bulk critical point. Using our results for both ^{2} and ^{2}, we estimate that in the limit $!_c$ both quantities have the limiting value $R = 0:90(5)$.

Table 1
A few results for β and for κ_e

	0.2275	0.2327	0.2391	0.3000	0.40236
	0.0146(1)	0.0319(1)	0.0555(1)	0.30284(8)	0.67988(6)
	0.240	0.275	0.330	0.35	0.37
$κ_e$	16.7(5)	4.65(4)	1.93(2)	1.52(2)	1.20(2)

Figure 1. Results for $σ^2$ and $κ^2$

In the theory of critical wetting, the quantity $ω(β) = 1/(4πσ^2)$ plays an important role. In a paper of Fisher and Wen [12] this quantity is estimated over a wide range of temperatures. A comparison of our data with their theoretical prediction will be published elsewhere [13].

When β approaches the roughening coupling $β_R$, Kosterlitz-Thouless theory states that $κ_e \to 2/π$. Using the estimates $β_R = 0.4074(3)$ [14], and $σ(β_e) = 0.3163$ (from the Pade that here certainly is reliable), we find a "KT value" of $σ^2$ which is 0.1572.

In order to demonstrate the efficiency of the Hasenbusch-Meyer algorithm we redid the surface width computation of Mon et al. [2] at $β = β_c = 0.8 × 0.2771$ on lattices of size $L × L × 27$, with $L = 32, 64, ..., 512$. We performed fits of the data using the ansatz

$$W^2 = \text{const} + \frac{κ_e}{2π} \ln L \qquad (11)$$

that is motivated by Kosterlitz-Thouless theory of a rough interface. When the $L = 32$ data were excluded, the fits where quite convincing. From our analysis we arrive at an estimate $κ_e = 4.3(2)$. This result is nicely consistent with the $κ_e$ as obtained from the renormalization group quantities A.

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