Numerical Investigation of the Interface Tension in the three-dimensional Ising Model

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Abstract

The interface tension in the three-dimensional Ising model in the low temperature phase is investigated by means of the Monte Carlo method. Together with other physically relevant quantities it is obtained from a calculation of time-slice correlation functions in a cylindrical geometry. The results at three different values of the temperature are compared with the predictions from a semiclassical approximation in the framework of renormalized $\phi^4$ theory in three dimensions, and are in good agreement with them.
1 Introduction

In various systems in statistical mechanics or in nature at temperatures $T$ below a certain critical temperature $T_c$ interfaces (domain walls) may be present, separating coexisting phases. The interface tension $\tau$ is the free energy per unit area of interfaces. It is an interesting quantity for various reasons. For numerical simulations of field theories in a phase with broken discrete symmetry finite volume effects are often dominated by tunneling $[1]$. The size of these finite volume effects is intimately related to the interface tension. Secondly, the interface tension is relevant for first order phase transitions, where it determines the nucleation rate.

For many binary systems the interface tension $\tau$ has been investigated experimentally as a function of the temperature $T$ $[2, 3, 4, 5]$. As $T$ increases towards $T_c$ the reduced interface tension

$$\sigma = \frac{\tau}{kT},$$

(1)

where $k$ is Boltzmann’s constant, vanishes according to the scaling law

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

(2)

where

$$t = \left| \frac{T - T_c}{T_c} \right|,$$

(3)

and $\sigma_0$ is the critical amplitude of the interface tension. Widom’s scaling law $[6, 7]$, $\mu = 2 \nu$, (4)

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

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

(5)

The experimental results $[7, 2, 3, 4]$ for the critical index $\mu$,

$$\mu = 1.26 \pm 0.01,$$

(6)

and for the critical exponent $\nu$ $[8, 9, 10]$, as well as the prediction from the renormalization group $[11]$,

$$\nu = 0.630 \pm 0.002,$$

(7)
are consistent with Widom’s law.

Other quantities, which are universal according to the scaling hypothesis [12, 13], are the dimensionless products of critical amplitudes

\[ R_+ = \sigma_0 (\xi_0^+)^2, \quad R_- = \sigma_0 (\xi_0^-)^2, \quad \] (8)

where \( \xi_0^+ \) and \( \xi_0^- \) are the critical correlation length amplitudes in the high-temperature and low-temperature phases, respectively.

On the theoretical side we dispose of two models in the relevant universality class, the Ising model and the \( \phi^4 \) field theory in three Euclidean dimensions. Early field theoretic calculations [14, 15] of \( R_- \) (and \( R_+ \)) in the framework of the \( \epsilon \)-expansion, where \( d = 4 - \epsilon \) is the number of dimensions of space, were in disagreement with the experimental results. The discrepancy could, however, be resolved by a calculation in renormalized field theory directly in three dimensions [16]. This calculation was performed by means of a semiclassical saddle-point expansion to one-loop order around the kink-solution. The semiclassical method yields an expression for the energy splitting between the two “vacua” due to tunneling in a finite volume, which involves the interface tension. For some quantities related to the energy splitting and the interface tension it yields definite predictions in terms of the renormalized parameters of the model (see below).

A similar development took place in the case of Monte Carlo simulations of the Ising model. First results for the interface tension [17], which were at variance with the (real) experiments, have been improved by recent numerical studies [18, 19], which made the discrepancy vanish.

A systematic numerical study of the interface tension and related objects, which would allow a comparison with the semiclassical approximation, was, however, completed only recently for the four-dimensional Ising model [20].

In this article we present the results of a Monte Carlo investigation of the three-dimensional Ising model. The interface tension is determined from the volume dependence of the energy splitting, a method that was introduced in [21]. Furthermore, masses and renormalized parameters are calculated, which are necessary for a comparison with the semiclassical formulae.

Let us add a remark about a controversy, which stems from work of Borgs and Imbrie [22]. They derive a formula for the asymptotic large volume behaviour of the energy splitting, which disagrees with the semiclassical result. Their result, however, is valid only at very low temperatures, where interfaces
are rigid. In three dimensions this low temperature region is separated from
the scaling region in the low temperature phase by the roughening transition
\[23\]. Above the roughening transition there are massless interface modes and
the results of \[22\] do not apply to the rough phase.

In four dimensions, however, there is a conflict between \[22\] and the
semiclassics, because of the absence of a roughening transition. The Monte
Carlo results of \[20\] are in favour of the semiclassical formula. Nevertheless
it might be possible that Borgs and Imbrie are right for very large volumes.
Namely, if one adopts the common assumption that the interface dynamics
is effectively described by a SOS-model or equivalently a discrete Gaussian
model, the results of Mack and Göpfert \[24\] suggest that in the scaling region
there is a very small mass in the interface dynamics, which only shows up in
the behaviour at very large volumes.

2 The three-dimensional Ising model

We consider the Ising model on a three-dimensional cubic lattice of cylindrical
geometry. This means that the lattice has a quadratic cross-section of area
$L^2$ in two directions and extends over $T$ lattice units in the third direction,
such that $L \ll T$. ($T$ is not to be confused with the physical temperature,
which does not appear any more from here on.) The Boltzmann factor is
denoted
\[ e^{-\beta \mathcal{H}}, \]
with
\[ \mathcal{H} = -\sum_x \sum_{\mu=1}^3 \phi_x \phi_{x+\hat{\mu}}, \quad \beta > 0, \]  
where $\hat{\mu}$ denotes the unit vector in the positive $\mu$-direction. The variables $\phi_x$
are associated with the lattice points and assume values $\phi_x = \pm 1$. They obey
periodic boundary conditions. The transfer matrix is denoted $e^{-H}$, where $H$
is the Hamiltonian in the language of quantum theory. The lowest eigenvalue
of $H$ is normalized to zero.

The three-dimensional Ising model in an infinite volume is known to pos-
sess a critical point at \[25, 26\]
\[ \beta_c = 0.221654 (6). \]
For $\beta > \beta_c$ the $\mathbb{Z}_2$-symmetry $\phi \to -\phi$ is spontaneously broken and the field acquires a non-zero vacuum expectation value, e.g.

$$\langle \phi_x \rangle = \pm v, \quad v > 0.$$  \hspace{1cm} (12)

In this phase the spectrum of the transfer matrix is doubly degenerate. In particular there are two ground states or “vacua” $|0_\pm\rangle$ with

$$\langle 0_+ | \phi(x) | 0_+ \rangle = v, \quad \langle 0_- | \phi(x) | 0_- \rangle = -v.$$  \hspace{1cm} (13)

On the other hand it is well known in statistical mechanics that spontaneous symmetry breaking does not occur in a finite volume. Let us consider a situation in which $L$ is finite. As a consequence of the Frobenius-Perron theorem applied to the transfer matrix \[27\] there is a unique ground state $|0_s\rangle$ symmetric under the reflection $\phi \to -\phi$, and the vacuum expectation value of the field vanishes. This means that the degeneracy of the infinite volume ground states $|0_\pm\rangle$ is lifted. Separated from the ground state $|0_s\rangle$ by a small energy splitting $E_{0a}$ there is an antisymmetric state $|0_a\rangle$, and if one decomposes these states as

$$|0_s\rangle \equiv \frac{1}{\sqrt{2}} (|0_+\rangle + |0_-\rangle) \quad |0_a\rangle \equiv \frac{1}{\sqrt{2}} (|0_+\rangle - |0_-\rangle),$$  \hspace{1cm} (14)

then $|0_+\rangle$ and $|0_-\rangle$ are states which go over into the degenerate vacua in the infinite volume limit.

The energy splitting $E_{0a}$ is due to tunneling between $|0_+\rangle$ and $|0_-\rangle$ in a finite volume. Its volume dependence was studied in \[28, 29\]. Their analysis is based on a picture of domains which extend over the spatial volume and cover certain intervals in time. Neighbouring domains with a different sign of the field are separated by domain walls, which can be considered as tunneling events. From this picture a prediction about the energy splitting of the form

$$E_{0a} \sim \exp \left\{ -\sigma L^2 \right\}$$  \hspace{1cm} (15)

is obtained, where $\sigma$ is the interface tension associated with the domain walls. One sees that tunneling effects vanish very rapidly with increasing volume.

The next higher states are the symmetric and antisymmetric one-particle states with energies $E_{1s}$ and $E_{1a}$, respectively. In the limit $L \to \infty$ they become degenerate too, and their energy defines the physical mass $m$. 
In a numerical simulation the low-lying spectrum of zero-momentum states can be obtained from correlations of time-slices
\[ S_t \equiv \frac{1}{L^2} \sum_x \phi_{x,t}, \quad x = (x, t). \] (16)
Let
\[ Z \equiv \text{Tr} e^{-TH} = 1 + e^{-TE_{0a}} + e^{-TE_{1s}} + e^{-TE_{1a}} + \ldots \] (17)
be the partition function. Then the vacuum expectation value of the product of timeslice field averages is given by
\[ \langle S_0 S_t \rangle Z \equiv \text{Tr} \{ S_0 e^{-tH} S_t e^{-(T-t)H} \} \]
\[ = v^2 \left[ e^{-tE_{0a}} + e^{-(T-t)E_{0a}} \right] + c_{01}^2 \left[ e^{-tE_{1a}} + e^{-(T-t)E_{1a}} \right] \\
+ c_{10}^2 \left[ e^{-(T-t)E_{0a} - tE_{1s}} + e^{-(T-t)E_{0a} - tE_{1s}} \right] \\
+ c_{11}^2 \left[ e^{-(T-t)E_{1a} - (T-t)E_{1s}} + e^{-(T-t)E_{1a} - (T-t)E_{1s}} \right] + \ldots \] (18)
where the matrix elements are defined as
\[ v \equiv \langle 0_s | S_t | 0_a \rangle \] (19)
\[ c_{01} \equiv \langle 0_s | S_t | 1_a \rangle \quad c_{10} \equiv \langle 1_s | S_t | 0_a \rangle \quad c_{11} \equiv \langle 1_s | S_t | 1_a \rangle . \] (20)
The field expectation value \( v \) and the energy splitting \( E_{0a} \) can be extracted from the \( t \)-dependence of \( \langle S_0 S_t \rangle \), if \( T \) and \( t \) are chosen suitably large. We define the connected time-slice correlation function in a finite volume by
\[ \langle S_0 S_t \rangle_c \equiv \langle S_0 S_t \rangle - \frac{v^2}{Z} \left( e^{-tE_{0a}} + e^{-(T-t)E_{0a}} \right) . \] (21)
Here one can use the approximation
\[ Z = 1 + e^{-TE_{0a}} \] (22)
for large enough \( T \). The susceptibility is given by
\[ \chi_2 \equiv L^2 \sum_t \langle S_0 S_t \rangle_c , \] (23)
and the second moment of the correlation function is defined by

\[ \mu_2 \equiv 3L^2 \sum_t \langle S_0 S_t \rangle_c \sin^2 \frac{\pi t}{T} \left( \frac{\sin^2 \frac{\pi}{T}}{1} \right)^{-1}. \]  

(24)

The correlation function of squared time-slices, \( \langle S_0^2 S_t^2 \rangle \), has an expansion similar to (18), from which the energies \( E_{1s} \) and \( E_{2s} \) can be obtained.

Near the critical point, where one is deep enough in the scaling region, the critical behaviour can be described in terms of the three-dimensional \( \phi^4 \) theory, which is in the same universality class. The quantities, which are usually handled in field theory, are defined differently from those, which are common in statistical physics. For the definition of the renormalized mass \( m_R \), the wavefunction renormalization factor \( Z_R \) and the renormalized field expectation value \( v_R \) we refer to [1]. The relation to the quantities introduced above is in three dimensions given by

\[ m_R^2 = \frac{6\chi_2}{\mu_2}, \quad Z_R = \frac{6\beta\chi_2^2}{\mu_2}, \quad v_R = \sqrt{\beta/Z_R} v. \]  

(25)

A suitably defined dimensionless renormalized coupling is

\[ u_R \equiv \frac{3}{v_R^2} \frac{m_R}{u_R}. \]  

(26)

The energy splitting \( E_{0a} \) can be calculated in a semiclassical approximation, which amounts to a saddle-point expansion around the classical kink solution of \( \phi^4 \) theory. The kink interpolates between the two field values at the minima of the potential and represents an interface separating regions with different local mean values of the field. The calculation including quadratic fluctuations around the kink solution has been done in [30] for \( d=4 \) dimensions and in [16] for the three-dimensional case. In three dimensions the result is

\[ E_{0a} = C \exp \left\{ -\sigma(L)L^2 \right\}, \]  

(27)

where \( \sigma \) is the interface tension, and

\[ C = \frac{\Gamma(3/4)}{\Gamma(1/4)} \sqrt{\frac{2}{u_R}} m. \]  

(28)
The interface tension has a negligible exponentially small \( L \)-dependence and the value at \( L = \infty \) is
\[
\sigma_\infty = 2 \frac{m^2}{u_R} \left( 1 - \frac{u_R}{4\pi} \left( \frac{39}{32} - \frac{15}{16} \log 3 \right) + \mathcal{O}(u_R^2) \right).
\] (29)

Since \( m \) is the inverse of the correlation length in the low temperature phase, we obtain an expression for the universal amplitude product
\[
R_- = \frac{2}{u_R^*} \left( 1 - \frac{u_R^*}{4\pi} \left( \frac{39}{32} - \frac{15}{16} \log 3 \right) + \mathcal{O}(u_R^*^2) \right),
\] (30)

where \( u_R^* \) is the value of \( u_R \) at the critical point. From a combination of various analytical results in the literature it can be estimated to be
\[
u_R^* = 15.1 \pm 1.3.
\] (31)

which yields
\[
R_- = 0.1024 \pm 0.0088
\] (32)

and
\[
C/m = 0.49 \pm 0.02
\] (33)

for \( \beta \to \beta_c \).

### 3 Monte Carlo calculation

We performed Monte Carlo simulations of the three-dimensional Ising model on lattices with an extension of \( T = 120 \) in the third direction. For the simulation the algorithm of Swendsen and Wang \[31\] was employed. Wolff’s one-cluster version \[32\], which usually performs better, was not used, since we wanted to take advantage of the improved estimators for four-point functions. Three different values of the inverse temperature \( \beta \) were taken, namely \( \beta = 0.2275, 0.2327 \) and \( 0.2391 \). The size \( L \) was varied in steps of 2 in the ranges 10–18, 8–14 and 4–10, respectively. From the correlation functions of time-slices and squared time-slices the field expectation value \( v \) and the energies \( E_{0a}, E_{1a}, E_{1s} \) and \( E_{2s} \) were obtained by means of fits to the \( t \)-dependence. Furthermore the susceptibility \( \chi_2 \) and the second moment \( \mu_2 \) have been calculated. The results for the energies are displayed in table 1.
The table also contains estimates for the physical mass $m$, which are obtained by weighted averages of $E_{1s}$ and $E_{1a}$ on the largest available lattices. For the $\beta$-value closest to the critical point the $L$-dependence of the low-lying spectrum is shown in figure 1.

For each value of $\beta$ the energy splittings have been fitted according to

$$E_{0a} = C \exp \left\{ -\sigma L^2 \right\}, \quad (34)$$

in order to get the interface tension and the prefactor $C$. The fits are displayed in figure 2 and the numerical results are collected in table 2.

The values for $\sigma$ are then fitted to the scaling law in both forms

$$\sigma = \sigma_0 |1 - \beta / \beta_c|^\mu \quad (35)$$

and

$$\sigma = \sigma_0 |1 - \beta_c / \beta|^\mu. \quad (36)$$

The results are

$$\mu = 1.22(1), \quad \sigma_0 = 1.29(4) \quad (37)$$

and

$$\mu = 1.28(1), \quad \sigma_0 = 1.64(5), \quad (38)$$

respectively. The fit (36) is drawn in figure 3. The corresponding fits for the physical mass, which is equal to the inverse correlation length $\xi$, yield

$$\nu = 0.61(5), \quad m_0 = 3.8(6) \quad (39)$$

and

$$\nu = 0.64(6), \quad m_0 = 4.3(7). \quad (40)$$

The differences are due to the fact that one is not close enough to the critical point, but the critical exponents are well consistent with the known values from the literature. Forming the universal amplitude ratio we obtain

$$R_\perp = 0.09(3), \quad (41)$$

in excellent agreement with the estimate (32).

From the correlation function of time slices the field theoretic quantities have been calculated too. The results are contained in table 3. The second moment $\mu_2$ has a relatively large error. This is due to the fact that it is
sensitive to the correlation function at larger distances, where the signal-to-
noise ratio is smaller. As a consequence also the estimates for $m_R$ and the
coupling $u_R$ are afflicted by large uncertainties. The numerical values for
$m_R$ are, however, well consistent with those for $m$, as expected from series
expansion results [33]. Furthermore the values for $u_R$ agree with the estimate
(31) within errors.

In order to compare with the semiclassical formulae we formed the ratiros $\sigma/m^2$ and $C/m$ from the measured values. The results are shown in
table 4. Although in the temperature range under consideration $\sigma$ and $C$
are varying by factors of 4 and 2, respectively, the dimensionless ratios are
nearly constant, supporting the semiclassical prediction. The corresponding
couplings $u_R$, calculated according to (29) and (28) are also shown. As the
table reveals the couplings obtained in this way are in good agreement with
each other for each value of $\beta$. They are also consistent with the measured
couplings as well as with the estimate (31).

4 Conclusion

The Monte Carlo simulation of the three-dimensional Ising model on a lattice
with cylindrical geometry allowed to determine the energy splitting $E_{0\alpha}$ in
a finite volume with an accuracy sufficient for a calculation of the interface
tension $\sigma$. The scaling law for $\sigma$ and for the inverse correlation length $m$ was
verified and the resulting amplitude product $R_-$ is in very good agreement
with an estimate based on a semiclassical approximation in the framework
of $\phi^4$ theory. The dependence of $\sigma$ and the prefactor $C$ on the renormalized
mass $m_R$ and on the renormalized dimensionless coupling $u_R$ predicted by
the semiclassical approximation to one-loop order is in agreement with the
results of the numerical simulation.

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versity of Münster.
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Table 1
The low-lying energies on lattices of size $L^2 \cdot T$. The physical mass $m$ in the last row is the weighted average of $E_{1s}$ and $E_{1a}$ on the largest available lattices.

|       | $E_{0a}$ | $E_{1s}$ | $E_{1a}$ | $E_{2s}$ | $m$  |
|-------|----------|----------|----------|----------|------|
| $\beta = 0.2275$ |          |          |          |          |      |
| $L = 10$ | 0.04334(8) | 0.42(4) | 0.69(6) | 1.4(4) |      |
| $L = 12$ | 0.0217(1)  | 0.36(4) | 0.55(3) | 1.0(2) |      |
| $L = 14$ | 0.00989(7) | 0.35(4) | 0.455(16) | 0.84(14) |   |
| $L = 16$ | 0.00400(7) | 0.38(5) | 0.410(13) | 1.0(2) |      |
| $L = 18$ | 0.00151(8) | 0.39(3) | 0.420(12) | 1.0(4) | 0.416(16) |  |
| $\beta = 0.2327$ |          |          |          |          |      |
| $L = 8$  | 0.0348(1)  | 0.54(4) | 0.90(15) | 1.4(2) |      |
| $L = 10$ | 0.01069(7) | 0.51(2) | 0.67(2) | 1.2(1) |      |
| $L = 12$ | 0.00253(10)| 0.54(2) | 0.606(20) | 1.1(2) |      |
| $L = 14$ | 0.00047(20)| 0.59(7) | 0.62(1) | 1.5(5) | 0.619(14) |  |
| $\beta = 0.2391$ |          |          |          |          |      |
| $L = 4$  | 0.174(1)   | 1.05(2) | 5(3)     | 1.8(3) |      |
| $L = 6$  | 0.0491(2)  | 0.74(7) | 1.35(9)  | 2.1(5) |      |
| $L = 8$  | 0.00990(3) | 0.70(6) | 0.86(2)  | 1.5(2) |      |
| $L = 10$ | 0.00128(6) | 0.79(5) | 0.808(16) | 2.0(6) | 0.806(20) |  |

Table 2
The interface tension $\sigma$ and the prefactor $C$ obtained from a fit of the $L$-dependence of $E_{0a}$ according to (34).

| $\beta$ | $\sigma$   | $\ln C$   | $C$    |
|---------|------------|-----------|--------|
| 0.2275  | 0.0150(1)  | -1.675(19)| 0.187(4) |
| 0.2327  | 0.0328(2)  | -1.260(13)| 0.284(4) |
| 0.2391  | 0.0572(2)  | -0.955(10)| 0.385(4) |
Table 3

Renormalized parameters determined from the numerical simulation.

| $\beta$  | $m$      | $m_R$   | $v_R$   | $Z_R$  | $u_R$   |
|----------|----------|---------|---------|--------|---------|
| 0.2275   | 0.416(16)| 0.44(05)| 0.262(30)| 0.80(19)| 19(7)   |
| 0.2327   | 0.619(14)| 0.62(12)| 0.34(06)| 0.71(27)| 16(9)   |
| 0.2391   | 0.806(20)| 0.80(32)| 0.40(16)| 0.65(52)| 15(18)  |

Table 4

The dimensionless ratios $\sigma/m^2$ and $C/m$ as obtained in the numerical simulation. The columns to the right of these ratios contain the coupling $u_R$ calculated from the ratio according to the semiclassical expressions (29) and (28), respectively.

| $\beta$  | $\sigma/m^2$ | $u_R$   | $C/m$  | $u_R$   |
|----------|--------------|---------|--------|---------|
| 0.2275   | 0.087(7)     | 17.1(1.0)| 0.450(20)| 18.0(1.6)|
| 0.2327   | 0.086(4)     | 17.2(0.6)| 0.458(12)| 17.4(0.9)|
| 0.2391   | 0.088(4)     | 16.9(0.6)| 0.477(13)| 16.1(0.9)|

Figure Captions

**Fig. 1:** The low-lying spectrum at $\beta = 0.2275$ as a function of the lattice size $L$.

**Fig. 2:** The logarithm of the energy splitting $E_{0a}$ versus the lattice cross-section $L^2$ for three values of the inverse temperature $\beta$. Also shown are the fits according to (34).

**Fig. 3:** The logarithm of the interface tension $\sigma$ versus $\ln(1 - \beta_c/\beta)$. Also shown is the fit according to the scaling law (36).