Finite-size effects in the rough phase of the 3d Ising model

Walter Selke∗
Institut für Theoretische Physik, RWTH Aachen University, Germany

Abstract
Using Monte Carlo simulations, finite-size effects of interfacial properties in the rough phase of the Ising on a cubic lattice with \( L \times L \times R \) sites are studied. In particular, magnetization profiles perpendicular to the flat interface of size \( L \times R \) are studied, with \( L \) being considerably larger than \( R \), in the (pre)critical temperature range. The resulting \( R \)-dependences are compared with predictions of the standard capillary-wave theory, in the Gaussian approximation, and with a field theory based on effective string actions, for \( L = \infty \).

Keywords: Ising model, Interface, Rough phase, Monte Carlo simulation

1. Introduction
In the three-dimensional Ising model, the interface roughening transition occurs at the temperature \( T_r \), well below the bulk critical temperature, \( T_c \). The interface separates two regions with, predominantly, oppositely oriented spins, \( S_i = +1 \) or \( S_i = -1 \), with \( i \) denoting the lattice sites. In the thermodynamic limit, at temperatures below \( T_r \), the sharp interface has a finite width, while above, \( T_r \), i.e. in the rough phase, the interface width diverges.

The existence of a roughening transition has been predicted about seventy years ago [1, 2]. A rather simple theoretical description is based on a Gaussian approximation of the energy needed for forming the area of the interface [3]. That description of the long-wavelength fluctuations of the interface is usually called the capillary-wave theory (CWT), see, e.g., the review by Gelfand and Fisher [4] and the fairly recent article by Köpf and Münster [5].

In this contribution, new Monte Carlo simulations related to the roughening transition in 3d Ising models will be presented. Pioneering articles on that transition have been published, especially, by Dietrich Stauffer and coauthors [6, 7]. Cubic lattices with \( L \times L \times R \) sites have been studied, where the, at \( T = 0 \), flat interface consists of \( L \times L \) sites. \( R \) has been fixed. Then, originally, the roughening transition has been found to take place at \( T_r/T_c \approx 0.56 \) [6]. Furthermore, increasing \( L \), the interface width, \( W_i \), has been observed to diverge, in the rough phase, logarithmically with \( L \). This behavior is closely related to the Kosterlitz-Thouless transition of the 2d XY model [6, 7, 8, 9].

More recently, numerical estimates for \( T_r \) and \( T_c \) have been improved. Nowadays, the, presumably, best estimates are \( k_B T_r/J = 2.4537... \) [10] and \( k_B T_c/J = 4.51152... \) [11]. Obviously, the first Monte Carlo estimate for the roughening transition [6] has been confirmed rather well.

In this article, finite-size effects in the rough phase of the 3d Ising model are studied. Again, we shall consider lattices with \( L \times L \times R \) sites. Now, however, the, at \( T = 0 \), flat interface comprises \( L \times R \) spins, with \( L \) being "considerably larger" than \( R \), in contrast to the situation outlined above. Accordingly, the aim will be to determine the \( R \)-dependence of the interface width \( W_i \). Numerical results will be compared to theoretical predictions on the \( R \)-dependence in the limit \( L = \infty \). On the one side, the finite-size behavior may be described in the framework of the Gaussian approximation of the CWT, on the other side, there are more sophisticated variants using concepts of string theory [12, 13].

The outline of the article is as follows: In Section 2, the model and the simulation method as well as related predictions of pertinent theories will be sketched. Then, numerical results will be presented and compared to the asymptotics suggested by the theories. Finally, conclusions will be given.

∗Corresponding author
Email address: selke@physik.rwth-aachen.de (Walter Selke)

Preprint submitted to Physica A

September 7, 2020
2. Model, method, and theoretical predictions

We study the nearest-neighbor Ising model with ferromagnetic couplings, $J$, between neighboring spins, where $S_i = +/−1$ at site $i$. We consider cubic lattices with $L \times L \times R$ spins in the $x$, $y$- and $z$-directions. The lattice constant is set equal to one. The interface is introduced by fixing the boundary spins in the top and bottom $x$-$y$-layers, each comprising $L \times L$ sites. In these two layers, at distance $R$, the spins are fixed in the state $-1$ for $x < 0$, while the spins are in the state $+1$ for $x > 0$. For $x = 0$, the boundary spins are left free, setting them formally equal to zero. At the other boundaries of the lattice, free boundary conditions are used. Thence, in the ground state, at $T = 0$, a flat interface, of area $L \times R$, runs between the axes $x = 0$ on the top and bottom layers, see [13].

Obviously, interesting properties of the interface follow from the magnetization profile $m(x)$ in the central $x$-$y$-layer, $z = 0$, of the lattice, taking also $y=0$. At $T = 0$, for the flat interface, $m(x)$ is a step function, with $m(x) = -1$ for $x < 0$, and $m(x) = 1$ for $x > 0$. A typical example for the magnetization profile in the rough phase is shown in Fig. 1, as obtained in Monte Carlo simulations.

Indeed, the magnetization profile, $m(x)$, plays a crucial role in the theories describing finite-size behavior for the interface of this model, in the case of $L = \infty$ and sufficiently large values of $R$.

In the CWT, the Hamiltonian is given by the change of the interface area due to long-wavelength fluctuations. Then, the important term depends on $\sqrt{1 + |m'(x)|^2}$. In the Gaussian approximation, this expression is replaced by the term in leading order of the Taylor expansion, being proportional to $m'(x)^2$. For the geometry discussed above, the magnetization profile, $m(x)$, is given by the error function

$$m(x) \propto \text{erf}(\eta x)$$

(1)

with $\eta \propto \sqrt{1/\ln R}$ at fixed temperature. Accordingly, the slope of $m'(x)$ at the origin $x=0$ is given by

$$m'(0) \propto \sqrt{1/\ln R}$$

(2)
The interface width, \( W_i \), follows from \( m(x) \) by the second moment of its derivative \( m'(x) \). Then, the finite-size behavior, as a function of the length \( R \), has the form

\[
W_i \propto \ln R
\]  
(3)

with the proportionality factor depending on temperature \([14]\).

A different \( R \)-dependence of the slope and the interface width has been predicted by a recent string theory \([13]\). This theory is supposed to be valid for \( R \) being much larger than the correlation length in the (pre)critical region of the model. In particular, one obtains

\[
m'(0) \propto \sqrt{1/R}
\]  
(4)

and

\[
W_i \propto R
\]  
(5)

To test the two conflicting theories, we do not concentrate on critical phenomena very close to the bulk transition, so that standard Metropolis Monte Carlo simulations seem to be suitable \([15]\). To compare simulation results with the theoretical predictions, \( L \) is chosen to be "considerably larger" than \( R \). As stated above, in these theories, \( L \) is assumed to be infinite, and the theories describe dependences on the distance \( R \).

Note, that previous Monte Carlo data, for magnetization profiles, \( m(x) \), as well as related energy profiles agreed nicely with predictions of the string theory \([13]\). However, a systematic simulation study of finite-size effects is still missing.

Specifically, we, mainly, performed Monte Carlo simulations at fixed temperature, \( k_B T/J = 4.2 \), i.e. at about 0.93 \( T_c \). We varied \( R \) from 3 to 125, with \( L \) increasing from 79 to 363. Typically, averages over at least four, up to eight independent runs were taken. The typical length of each run was \( 10^6 \) to \( 10^7 \) Monte Carlo steps per site. We computed magnetization profiles, \( m(x) \), along the axis \( y = z = 0 \). Then the resulting slope at \( x = 0 \), \( m'(0) \), and the interface width, \( W_i \), were plotted against the \( R \)-dependences suggested by the two theories, see equations (2-5).

3. Results

To ensure that comparison of the simulation data to the theories assuming \( L \) being infinite, is reasonable, we checked the dependence of the slope \( m'(0) \) on the ratio \( r = R/L \) for various fixed values of \( R \). For \( R \) ranging from 3 to 51, the slope was observed to increase monotonically when decreasing \( r \). When increasing \( R \), the maximum, corresponding, presumably, to the case \( r = 0 \), was reached already at fairly large ratios. Indeed, for \( R > 7 \), the maximal slope was approached closely already for \( r \) being about 0.3-0.35 (then, \( R \) is larger than the bulk correlation length of the Ising model at the chosen temperature, \( k_B T/J = 4.2 \)). In this way, we may quantify the requirement, stated above, for comparing simulation results to the theories, that \( L \) is "considerably larger" than \( R \). In fact, all the data shown in Figs. 2 and 3 satisfy this condition. In fact, for \( R < 11 \), the ratio \( r \) was chosen to be even much smaller than 0.3.

Results of the systematic Monte Carlo simulations for the interface width, \( W_i \), and for the slope of the magnetization profile at the origin, \( m'(0) \), are depicted in Figs. 2 and 3. The focus is, at \( k_B T/J = 4.2 \), on the \( R \)-dependence, choosing sufficiently large values of \( L \), to allow for comparison with the capillary wave theory, in the Gaussian approximation, and with the string theory.

The two theories predict different asymptotics for the \( R \)-dependences of interfaces in the limit \( L = \infty \), see equations (2-5). Accordingly, we analyzed both the slope of the magnetization profile at the origin, eqs. (2) and (4), as well as the interface width, eqs. (3) and (5). Due to the discrete lattice structure, the slope may be approximated by

\[
m'(0) = (m(1) - m(-1))/2
\]  
(6)

The interface width may be defined by

\[
W_i = F \sum_{x} m'(x + 1/2) \times (x + 1/2)^2 / \sum_{x} m'(x + 1/2)
\]  
(7)

with \( m'(x + 1/2) = m(x + 1) - m(x) \). The sums run between the two plateaus of the magnetization profile, where \( m' \) approaches zero, see figure 1. Of course, the regions close to the (free) boundaries are ignored, to avoid their influence.
Figure 2: Slope of the magnetization profile at the origin, $m'(0)$, equation (6), plotted against $1/\sqrt{\ln R}$ (circles) and against $1/\sqrt{R}$ (squares). $R$ varies from 3 to 125 with the ratio $r = R/L$ being always smaller than 0.35.

Figure 3: Interface width $W$, equation (7), plotted against $\ln R$ (circles) and $R$ (squares), for the same lattices as in figure 2.
The simulation results for the slope and for the interface width are depicted in Figs. 2 and 3. In both cases, the $R$-dependence has been plotted against the asymptotic forms suggested by the capillary wave and the string theories, as discussed above.

For the slope $m'(0)$, figure 2, we observe, for sufficiently large distances $R$, linear dependences both in $1/\sqrt{\ln R}$, as predicted by CWT, as well as in $1/\sqrt{R}$, as predicted by the string theory. However, simple extrapolation to $R = \infty$ would give only in case of the scale proposed by the CWT a vanishing slope in the limit $R = \infty$, while in case of the scale according to the string theory, a limiting slope of about 0.1 seems to result, when extrapolating the simulation data. This finding will be addressed again later in this section.

The interface width $W_i$ is depicted in figure 3, plotted against $\ln R$, in accordance with the CWT, and against $R$, in accordance with the string theory. Here, a linear dependence seems to set in already at moderate values of $R$, when testing the CWT. On the other hand, the simulation data for $W_i$ appear to approach, if at all, the asymptotic form, suggested by the string theory, only for larger values of $R$. Again, the discussion on this topic will be postponed to the Conclusions. Note that similar behaviors have been found when estimating the interface width by the string theory. Most importantly, the string theory is expected to hold, asymptotically, for large values of $R$, according to the string theory. Here, a linear dependence seems to set in already at moderate values of $R$. Again, the discussion on this topic will be postponed to the Conclusions.

Note that a less elaborate MC simulation study for lattices of moderate sizes, ranging from $R = 7$ up to 51, in the rough phase at a lower temperature, $k_B T/J = 3.4$, shows good agreement with the CWT, both for the slope of the magnetization profile at the origin and for the interface width, see, equations (2) and (3). Interestingly, in the string case, the magnetization slope tends to a rather large non-zero value, of about 0.35, when extrapolating the MC data linearly to the limit $R = \infty$, compare to figure 2.

On the other hand, we performed preliminary simulations at a temperature closer to $T_c$, $k_B T/J = 4.4$, with $R$ ranging from 15 to 45 lattice units. At this temperature, a straightforward linear extrapolation of the MC data for the magnetization slope, plotted versus $1/\sqrt{R}$, leads to a very small value, of less than 0.01, in the limit $R = \infty$. In fact, this behavior may signal possible agreement with the string theory. Of course, more detailed computations, possibly, even closer to $T_c$ and for sufficiently large lattices, are desirable.

4. Conclusions

Systematic and rather extensive Monte Carlo simulations, especially, at $k_B T/J = 4.2$, have been performed to study finite-size effects of interface properties in the rough phase of the three-dimensional Ising model. The interface properties are related to the magnetization profile $m(x)$.

Lattices of $L \times L \times R$ sites are considered, with flat interfaces being of size $L \times R$. Simulation results are compared to predictions of two theories, the standard capillary wave theory, CWT, and a string theory. These theories, in the limit of $L = \infty$, lead to different asymptotics of finite-size dependences on $R$. According to the string theory, in the (pre)critical regime, rather unusual finite-size effects, for sufficiently large distances $R$, may occur.

In particular, we studied the slope of the magnetization profile in the center of the interface, $m'(0)$, as well as the interface width, $W_i$. For both quantities, the finite-size dependence, of $R$, agrees quite well with the predictions of the CWT for a wide range of values of $R$. At first sight, more pronounced deviations of the simulation data from the asymptotics following from the string theory are observed. Nevertheless, one has to be cautious in ruling out that theory. Most importantly, the string theory is expected to hold, asymptotically, for large values of $R$, in the (pre)critical regime, i.e. below, but sufficiently close to $T_c$. Thence, further simulations at higher temperatures seem to be desirable. Presumably, numerical algorithms reducing critical slowing down, in particular, cluster-flip updates, will be useful.

In addition, both theories are based on continuum descriptions. In contrast, in the Monte Carlo simulations, discrete lattices are studied.

In any event, open questions remain. In particular, the connection between the two theories needs to be clarified. Furthermore, the role of temperature, in the rough phase below the critical point, by going closer to $T_c$, should be elucidated.
Acknowledgements

Useful comments by G. Münster are gratefully acknowledged. I gladly remember numerous inspiring and helpful discussions with Dietrich Staußer, for about four decades. DS worked successfully on a wide range of topics, starting in traditional Statistical Physics, using various numerical and analytic methods. He liked to communicate, in a clear and humorous way, his profound insights to experts as well as to beginners.

References

References

[1] W. K. Burton, and N. Cabrera, Discuss. Faraday Soc. 5, 33, 1949
[2] W. K. Burton, N. Cabrera, and F. C. Frank, Philos. Trans. R. Soc. Lond. 243A, 299, 1951
[3] F. P. Buff, R. A. Lovett, and F. H. Stillinger, Phys. Rev. Lett 15, 621, 1965
[4] M.P. Gelfand and M. E. Fisher, Physica A 166, 1, 1990
[5] M. H. Köpf and G. Münster, J. Stat. Phys. 132, 417, 2008
[6] E. Bürkner and D. Stauffer, Z. Phys. B, 53, 241, 1983
[7] K. K. Mon, D. P. Landau, and D. Stauffer, Phys. Rev. B 42, 545, 1990
[8] J. M. Kosterlitz and D. Thouless, J. Phys C 6, 1181, 1972
[9] K. K. Mon, S. Wansleben, D. P. Landau, and K. Binder, Phys. Rev. Lett 60, 708, 1988
[10] M. Hasenbusch, S. Meyer, and M. Pütz, J. Stat. Phys. 85, 383, 1996
[11] A. M. Ferrenberg, J. Xu, and D. P. Landau, Phys. Rev. E 97, 043301, 2018
[12] M. Caselle, R. Fiore, F. Gliozzi, M. Hasenbusch, K. Pinn, and S. Vinti, Nucl. Phys.B 432, 590, 1994
[13] G. Delfino, W. Selke, and A. Squarcini, Nucl. Phys. B 958, 115139, 2020
[14] M. Caselle, F. Gliozzi, U. Magna, and S. Vinti, Nucl. Phys.B 460, 397, 1996
[15] D. P. Landau and K. Binder, “A Guide to Monte Carlo Simulations in Statistical Physics”, Cambridge University Press, 2014