Numerical simulations of a two-dimensional lattice grain boundary model

A. Jaster, H.H. Hahn

Institut für Theoretische Physik, TU Braunschweig, Mendelssohnstr. 3, D-38106 Braunschweig, Germany

May, 1997

Abstract

We present detailed Monte Carlo results for a two-dimensional grain boundary model on a lattice. The effective Hamiltonian of the system results from the microscopic interaction of grains with orientations described by spins of unit length, and leads to a nearest-neighbour interaction proportional to the absolute value of the angle between the grains. Our analysis of the correlation length $\xi$ and susceptibility $\chi$ in the high-temperature phase favour a Kosterlitz-Thouless-like (KT) singularity over a second-order phase transition. Unconstrained KT fits of $\chi$ and $\xi$ confirm the predicted value for the critical exponent $\nu$, while the values of $\eta$ deviate from the theoretical prediction. Additionally we apply finite-size scaling theory and investigate the question of multiplicative logarithmic corrections to a KT transition. As for the critical exponents our results are similar to data obtained from the XY model, so that both models probably lie in the same universality class.

1 Introduction

Phase transitions in two-dimensional systems with continuous symmetry are of great interest since many years. In these systems conventional long-range order at non-zero temperature cannot occur [1]. However, two-dimensional particle systems or the XY model are characterized at low temperatures by quasi-long-range order, while the high-temperature phase is disordered. The critical behaviour of the models depends on the dimension of the order parameter. For the two systems mentioned the order parameter dimension is two. Physical realizations of two-dimensional $O(2)$ symmetric systems are films of liquid helium or superconductive layers.

The XY model provides a simple model of a system with continuous symmetry. For the phase transition numerical studies favour a Kosterlitz-Thouless-like [2] behaviour. The KT mechanism is based on a topological defect (called vortex) unbinding scenario. In the low-temperature region vortices are bound in pairs. The dominant excitations are spin
waves, which destroy long-range order. Increasing the temperature leads to an unbinding of vortex pairs. The theory predicts a continuous transition from the quasi-long-range phase to the disordered phase derived from renormalization group treatment.

Particle systems are characterized by two order parameters related to different topological defects. Therefore, for the melting transition additional complications arise. There are several theoretical approaches for this transition. Halperin and Nelson \[3\] as well as Young \[4\] enhanced the ideas of Kosterlitz and Thouless. The KTHNY theory deals with a dislocation unbinding mechanism, which is responsible for the melting transition, and a disclination transition, which destroys the nearest-neighbour-bond orientation. An alternative scenario has been proposed by Chui \[5\]. He presented a theory via spontaneous generation of grain boundaries, i.e. collective excitations of dislocations. He found that grain boundaries may be generated before the dislocations unbind if the core energy of dislocations is sufficiently small, and predicted a first-order transition.

Another possibility to study two-dimensional melting is the simulation of the defect system itself. Saito performed Monte Carlo simulations of dislocation vector systems \[6\] and found that for systems with large dislocation core energy unbinding of dislocation pairs causes a continuous phase transition, while small core energies produce a first-order transition by formation of grain boundaries.

Patashinskii \[7\] proposed a model, which can be seen as a mesoscopic lattice model for grain boundaries. The energy per unit length of a boundary between two grains with small angle $\Delta \phi = \phi - \phi'$ is proportional to the absolute value of $\Delta \phi$. A simple ansatz for the description of the interaction of grains is then given by putting them on a square lattice with nearest-neighbour interaction proportional the absolute value for small lattice gradients. The orientation of the grains is described by spins of unit length \( \vec{s}(x) = (\cos \phi(x), \sin \phi(x)) \). Therefore Patashinskii used a Hamiltonian of the form

\[
H = \beta \sum_{<xx'>} \left| \sin \frac{N}{2} (\phi(x) - \phi(x')) \right| .
\]  

The number $N$ is related to the symmetry of the system. For example, particle systems with a hexagonal symmetry are described by $N = 6$. However, the partition function is essentially independent of $N$. Therefore we neglected this parameter and used angles of range $0 \leq \phi(x) < 2\pi$. Also, we used the simplified model

\[
H = \beta \sum_{<xx'>} |\phi(x) - \phi(x')| , \quad -\pi < \phi(x) - \phi(x') \leq \pi
\]  

for numerical simulations, since (at least in the case of a continuous phase transition) only the behaviour for small $\Delta \phi$'s is relevant. This coincides with an XY model with the negative cosine replaced by its absolute value. In this paper we try to determine the order and mechanism of the phase transition of this model.

The KT scenario predicts an exponential singularity for the correlation length

\[
\xi(t) = a_\xi \exp \left( b_\xi t^{-\nu} \right),
\]  

and the susceptibility $\chi$

\[
\chi(t) = a_\chi \exp \left( b_\chi t^{-\nu} \right)
\]  

Note
if \( t = \beta_c - \beta \ \downarrow 0 \), while the specific heat \( C_V \) should not show any divergent behaviour. The critical exponent \( \eta \) defined by

\[
\chi \sim \xi^{2-\eta},
\]

and the critical exponent \( \nu \) are given by

\[
\nu = \frac{1}{2}, \quad \eta = \frac{1}{4},
\]

while \( b_\xi \) is a non-universal constant and \( b_\chi = (2 - \eta) b_\xi \). An alternative approach is a conventional second-order behaviour with power-law singularities of

\[
\xi(t) = a_\xi t^{-\nu}
\]

and

\[
\chi(t) = a_\chi t^{-\gamma}.
\]

In the following we analyze our extensive Monte Carlo results to answer the question of kind and order of the phase transition of the grain boundary model.

## 2 Simulations

### 2.1 Algorithms and measurement

For the simulations we used a combination of the Metropolis, over-relaxation \[8, 9\] and cluster \[10, 11\] algorithm, depending on the temperature and size of the lattice. The study was carried out on lattice sizes of \( L^2 = 60^2, 120^2, 240^2, 480^2 \) and \( 960^2 \) with periodic boundary conditions.

For each simulation we measured the energy, specific heat, ‘magnetization’, susceptibility, fourth-order cumulant and the zero momentum correlation function (for a definition see eq. (12) below). In doing so, we used conventional estimators for all observables. Additional improved estimators \[12\] were measured for the susceptibility and correlation function. Typically, errors were of the order of 1% or less.

For the calculation of the specific heat we used two different ways: on one hand we measured the fluctuations in the energy per point

\[
C_V = \beta^2 L^2 (\langle e^2 \rangle - \langle e \rangle^2)
\]

on the other hand we compute the derivative

\[
C_V = -\beta^2 \partial e / \partial \beta.
\]

We find that both methods give consistent results as shown in fig. \[\text{fig}\]. Except for the smallest lattice the data do not show any significant finite-size effects. As one can see the specific heat develops a smooth peak at an inverse temperature below the transition point \( \beta_c \approx 0.83 \). At the transition point the energy and the specific heat stay finite and
show no divergent behaviour. This is consistent with a KT-like transition and makes a first- or second-order transition unlikely.

The magnetic susceptibility was calculated from fluctuations in the magnetization per point

$$\chi = L^2 \langle \vec{m}^2 \rangle, \quad \vec{m} = \frac{1}{L^2} \sum_{x,y} \vec{s}(x,y)$$

in the conventional manner and using improved estimators. Finite-size effects were studied by comparing data on different lattice sizes. We find that for correlation lengths $\xi < L/7$ no lattice size dependence of $\chi$ within the statistical errors can be seen.

In the high-temperature phase the correlation length was extracted from the 'zero momentum' spin-spin correlation function

$$\Gamma_s(x) = \langle \vec{s}(x) \cdot \vec{s}(0) \rangle, \quad \vec{s}(x) = \frac{1}{L} \sum_y \vec{s}(x,y)$$

by fitting the data with a single $\cosh$ or $\cosh + \text{const}$ in the interval $x_0 \leq x \leq L/2$. Most of the time, constant contributions were negligible, because they are of order $\exp(-L/\xi)$. 

Figure 1: Specific heat as a function of $\beta$. Full symbols stand for the calculation by numerical differentiation, open symbols denote the measurement of energy fluctuations.
To determine the influence of 'excitations' (smaller eigenvalues of the transfer matrix), we compared the results for different minimal distance $x_0$. The correlations are always dominated by the lowest state of the transfer operator 'Hamiltonian', so that we had to omit only few points. As for the susceptibility we used conventional and improved estimators. The latter have substantially smaller statistical errors, because only positive terms contribute to the correlation function. For $\beta > \beta_c$ it is expected that the long distance behaviour of the spin-spin correlation function is given by a power-law decrease with a critical exponent $\eta$ which is a function of $\beta$, but we made no investigations to this point.

### 2.2 Numerical results in the high-temperature phase

In the following we will analyze the critical behaviour of $\xi$ and $\chi$. Therefore, we have performed least square fits with three different forms (according to eqs. (3) and (7)). In the first case we used a four-parameter Kosterlitz-Thouless fit (KT4), i.e.

$$\ln(\xi) = a + b t^{-\nu},$$  \hspace{1cm} (13)

with $\beta_c = \beta + t$ as the fourth parameter. In the second case the value of $\nu$ was fixed to 0.5 (KT3). Assuming a power-law behaviour of the divergence we obtained the third case:

$$\ln(\xi) = a - \nu \ln(t).$$ \hspace{1cm} (14)

Systematic errors had been estimated by varying the range of points to be fitted and by replacing $t = \beta_c - \beta$ by $t = T - T_c$. We used data subsets consisting of all points with $6 < \xi < L/7$ and $12 < \xi < L/7$, respectively\[^1\]. This corresponds to $0.67 \leq \beta \leq 0.78$ (20 points) and $0.72 \leq \beta \leq 0.78$ (15 points). Errors for the fitted parameters were computed by performing fits on data sets to a Gaussian distribution of $\xi(\beta)$ with variance $\Delta \xi(\beta)$. All calculations were performed correspondingly for $\chi$.

Our results are summarized in table 1. Additionally one example is plotted in fig. 2. One observes that the KT like fits look consistent (except one of the KT3 fits for $\xi(\beta)$) and that both types always give a similar $\chi^2$ per degree of freedom (dof). The influence of the lower bound of the fitted interval is small. This situation changes for the power-law fits. The different intervals yield large changes in the fitted parameter. Also, PL fits have always larger $\chi^2$/dof than the KT fits. The data for the correlation length make a power-law divergence very unlikely.

Taking $\nu$ as a free parameter (KT4) results in large errors. This situation is similar as in the XY model \[^3,\,4\]. The reason is that in the four-parameter space a valley for $\chi^2$ exists, which is narrow in three dimensions, but flat in the fourth. The different fits with $\nu$ as a free parameter yield the estimate

$$\nu = 0.46(7).$$ \hspace{1cm} (15)

Holding $\nu$ or $T_c$ fixed leads to a clear minimum and much smaller errors in the remaining parameters. From the $\beta_c$'s of the three-parameter Kosterlitz-Thouless fits and the power-law fits we got the following values:

$$\beta_{c,\text{KT3}} = 0.8354(20),$$ \hspace{1cm} (16)

\[^1\]There is one exception: for the point $\beta = 0.7725$ we also got $L/\xi \approx 480/69.2 \approx 6.94$.\[5\]
Figure 2: The curves shown are the best fit for a Kosterlitz-Thouless behaviour with fixed $\nu$ (dotted) and a power-law ansatz (dashed). We used all correlation lengths $\xi > 6$. Statistical errors are too small for a visualization. The critical values of $\beta$ are visualized by vertical lines.

$$\beta_{c,PL} = 0.8079(30) .$$ \hspace{1cm} (17)  

We further analyzed our data by investigating the relation between $\chi$ and $\xi$. To check the validity of eqn. (16) we plot $\ln(\chi/\xi^{7/4})$ versus $\ln(\xi)$. For the predicted KT value $\eta = 1/4$ we should see a horizontal line. A different value of $\eta$ would correspond to a straight line of non-zero slope. Indeed, fig. 3 shows a negative slope, but with decreasing absolute value for increasing $\xi$. Performing straight line fits for the points $\xi > 12$ results in an estimate of

$$\eta = 0.270(3) .$$ \hspace{1cm} (18) 

For the points $\xi > 50$ we got $\eta = 0.259(17)$. The difference to the theoretical value can perhaps be explained by logarithmical corrections as discussed later.

It should be noted that the values of the critical exponent $\nu = 0.48(10)$ and $\eta = 0.267$ of the XY model in Villain’s formulation \[14\] (calculated with same methods) coincide with our grain boundary model within statistical errors. Also, the behaviour of $\ln(\chi/\xi^{7/4})$ as a function of $\ln(\xi)$ (fig. 3) is qualitatively the same in both cases. Hence it looks likely
Table 1: Best fit parameters for the critical behaviour of the correlation length and susceptibility. For $\xi > 6$ we have fitted 20 points in $0.67 \leq \beta \leq 0.78$. In the case $\xi > 12$ we used 15 points in the range $0.72 \leq \beta \leq 0.78$. 

|       | $\xi > 6$ | $\xi > 12$ | $\xi > 6$ | $\xi > 12$ | $\xi > 6$ | $\xi > 12$ |
|-------|-----------|------------|-----------|------------|-----------|------------|
|       | KT4       | KT3        | PL        |             |           |             |
| $\ln(a)$ | -3.62(33) | -2.92(88)  | -2.08(1)  | 0.176(1)   | 0.148(2)  |
| $b$     | 2.88(28)  | 2.30(73)   | 1.62(1)   | 1.59(1)    |           |
| $\beta_c$ | 0.8295(12)| 0.8323(36) | 0.8382(2) | 0.8373(3)  | 0.8097(1) | 0.8118(2)  |
| $\nu$   | 0.350(33) | 0.403(71)  | 0.5       | 0.5        | 1.816(3)  | 1.901(6)   |
| $\chi^2$/dof | 1.10     | 1.17       | 3.37      | 1.22       | 28.41     | 6.59       |

that the grain boundary model is in the same universality class as the XY model. Also, a detailed comparison indicates a faster convergence to the KT behaviour for the lattice grain boundary model than for the XY model in Villain’s formulation. The same analysis for the XY model in the cosine form yields non-unique results, since the data of [13, 15] have larger statistical errors.

### 2.3 Numerical results at the transition point

We now come to the simulations near the transition point. In the following we will concentrate on the fourth-order cumulant

$$U = 1 - \frac{\langle \vec{m}^4 \rangle}{3\langle \vec{m}^2 \rangle^2}$$

and the susceptibility. At the transition point finite-size scaling (FSS) implies scale invariance of $U$ and $\chi \sim L^{2-\eta}$ for large enough lattices. We use this FSS behaviour to locate $\beta_c$. For these simulations we used additional lattices of size $L^2 = 36^2$. 

7
Figure 3: Test of the scaling relation $\chi \sim \xi^{7/4}$. The tendency to decrease implies $\eta > 1/4$.

At the transition point the susceptibility should diverge with the size of the system as

$$\chi \sim L^{2-\eta}.$$  \hspace{1cm} (20)

For $\beta > \beta_c$ $\eta$ is a function of the temperature. For $\beta$’s below the transition point, one has to take corrections for finite correlation lengths of the order $O(L/\xi)$ into account. In fig. we plot $\ln(\chi/L^{7/4})$ versus $\ln(L)$ for three different $\beta$’s near the transition point. The slope gives the deviation from $\eta = 1/4$. We extracted the values of $\eta$ from linear fits of the asymptotic behaviour. Our results are collected in table 2. Obviously, a requirement of $\eta = 0.25$ yields $\beta_c \approx 0.826$. Since there is a tendency of the slope to decrease with

| $\beta$ | $\eta$ | $\chi^2$/dof | used lattices |
|--------|--------|--------------|--------------|
| 0.82   | 0.2663(13) | 0.89      | $L = 120 - 480$ |
| 0.825  | 0.2535(10)  | 2.91      | $L = 120 - 960$ |
| 0.83   | 0.2404(7)   | 0.01      | $L = 60 - 480$ |
| 0.84   | 0.2242(13)  | 1.49      | $L = 60 - 240$ |
larger lattices, the real scale invariance may take place at larger inverse temperatures. On the other hand, with $\beta_{c,KT3} \approx 0.836$ we got an $\eta$ which is about 8% below the theoretical value. Again this situation is similar as in the XY model [13, 14].

Our results for the dependence of $U$ on the lattice size are shown in fig. 5. Apart from the fact that the statistical errors are larger, we get a similar estimate as before. Also the slopes of $\ln(\chi/L^{7/4})$ and of $U$ both decrease with increasing $L$. Therefore, the value of $\beta_c$ can be taken as a lower bound of the large $L$ limit. If we compare this value with those of the KT and PL fits (eqn. (16) and (17)) we find that $\beta_{c,KT}$ is in better agreement than $\beta_{c,PL}$. This is an additional hint favouring a KT transition.

2.4 Logarithmic corrections to KT scaling laws

Assuming an exponential divergence as predicted by Kosterlitz and Thouless, one can ask for corrections of the scaling behaviour of $\xi$ and $\chi$. The renormalization group analysis of KT yields the following multiplicative corrections to eqn. (5):

$$\chi \sim t^r \xi^{2-\eta} , \quad r = -\frac{1}{16} .$$  \hspace{1cm} (21)

In the following we will analyze the data under the assumption that $\nu = 1/2, \eta = 1/4$ and determine if logarithmical corrections can explain the appearing discrepancies from
Figure 5: Finite-size scaling of the cumulant in the vicinity of the transition point.

the leading scaling behaviour. Therefore in fig. 6 we plotted \( \ln(\chi/\xi^{7/4}) \) as a function of \( -\ln(t) = -\ln(\beta_c - \beta) \), where we have taken \( \beta_c = 0.8354 \). The data are consistent with a straight line assumption, but from the slope (for the points \( \xi > 6 \)) we obtained

\[
    r = 0.070(5),
\]

which is completely different from the theoretical value. For the interval \( \xi > 12 \) we got \( r = 0.056(9) \). This means that the value of \( r \) decreases, so that we probably have not reached the scaling region. On the other hand a different \( \beta_c \) results in only small changes of \( r \).

Alternatively one can also try to replace \( -\ln(t) \) by \( 2\ln(\ln(\xi)) \) in fig. 6, as it follows from eqn. (3). This has the advantage, that no information about \( \beta_c \) is needed. It is clear that the relation is only fulfilled in the limit \( t \to 0 \), where \( b_t t^{-\nu} \gg |\ln(a \xi)| \). For the actual values of \( \beta \) this is not the case, as can be calculated using the parameters of table 1. Nevertheless one gets a linear behaviour which leads to \( r = 0.043(3) \) (\( \xi > 6 \)) and \( r = 0.036(6) \) (\( \xi > 12 \)), respectively. All data are summarized in table 3.

A different approach to estimate \( r \) is based one FSS. At the transition point (\( \xi \gg L \)) one expects

\[
    \chi \sim (\ln(L))^{-2r} L^{2-\eta}.
\]
Figure 6: Logarithmic corrections to the scaling of $\chi \sim \xi^{7/4}$. The slope yields $-r$. The dashed line results from a fit of all points with $\xi > 6$, i.e. $-\ln(\beta_c - \beta) > 1.77$.

In fig. 7 we show the data at $\beta = 0.83 \approx \beta_c$. Indeed we can observe the predicted linear behaviour. From the slope we obtain

$$r = -0.0233 (10).$$

Although the value is closer to the theoretical one, it is still in disagreement with it. A higher (lower) value of $\beta$ would result in a decrease (increase) of $r$. At $\beta = 0.84$ we got $r = -0.059(4)$.

The analysis for multiplicative corrections in the XY model yields similar results [16, 17], i.e. positive values of the order $O(0.05)$ from the data of the high-temperature phase and a negative value of approximate $-0.03$ from finite-size scaling.

## Conclusions

We presented a detailed Monte Carlo study of a two-dimensional grain boundary model on the lattice. The investigations were performed in the high-temperature phase and near the phase transition point.

The behaviour of the specific heat as a function of the inverse temperature $\beta$ was characterized by a smooth peak at an inverse temperature below the critical value. Moreover
Table 3: Values of the logarithmic correction exponent $r$ obtained from different methods.

| method                              | $r$     | $\chi^2$/dof | points |
|-------------------------------------|---------|--------------|--------|
| $\ln(\chi/\xi^{7/4})$ vs. $\ln(\beta_c - \beta)$ | $\xi > 6$ | 0.070(5)    | 0.86   | 20     |
|                                     | $\xi > 12$ | 0.056(9)   | 0.57   | 15     |
| $\ln(\chi/\xi^{7/4})$ vs. $\ln(\ln(\xi))$ | $\xi > 6$ | 0.043(3)    | 0.67   | 20     |
|                                     | $\xi > 12$ | 0.036(6)   | 0.56   | 15     |
| $\ln(\chi/L^{7/4})$ vs. $\ln(\ln(L))$ | $\beta = 0.83$ | -0.0233(10) | 0.26   | 5      |
|                                     | $\beta = 0.84$ | -0.059(4) | 4.20   | 3      |

for lattices of $L = 120$ or larger no finite-size effects were seen. This is consistent with the KT scenario.

In the high-temperature phase we examined the dependency of the correlation length and susceptibility on $\beta$ and $T$. We showed that the data are always in agreement with a KT-like divergence. The critical exponent $\nu$ was estimated as $\nu = 0.46(7)$. In all cases fits with a power-law divergence are characterized by a larger $\chi^2$/dof than the corresponding KT fit. The exponent $\eta$ was derived from the relation of $\xi$ and $\chi$ for $\beta \to \beta_c$. We got $\eta = 0.270(3)$.

The simulations in the vicinity of the transition point were used to measure the finite-size scaling of the fourth-order cumulant and susceptibility. The resulting estimates of $\beta_c$ are closer to the value from the KT fits than to the estimate from the PL fits. Deviations may be explained by the fact that the lattices used are still too small.

Additionally we discussed an attempt to explain differences of the critical exponent $\eta$ from the predicted KT values by multiplicative corrections. We showed that both finite-size scaling at $\beta_c$ and simulations in the high-temperature phase are consistent with such an ansatz. However the values of $r$ are inconsistent and far from the theoretical value $r = -1/16$. As before the reason might be too small lattice sizes.

A comparison of our results showed that the data are in accordance with the ones of the XY model. The universal critical exponents agree within statistical errors, while multiplicative corrections are qualitatively the same. We take this as evidence that both models lie in the same universality class.

References

[1] N.D. Mermin, H. Wagner, Phys. Rev. Lett. 17 (1966) 1133.

[2] J.M. Kosterlitz, D.J. Thouless, J. Phys. C 6 (1973) 1181; J.M. Kosterlitz, J. Phys. C 7 (1974) 1046.

[3] B.I. Halperin, D.R. Nelson, Phys. Rev. Lett. 41 (1978) 121.

[4] A.P. Young, Phys. Rev. B 19 (1979) 1855.
Figure 7: Logarithmic corrections to the finite-size scaling of the susceptibility near $\beta_c$. We derived $r$ from the slope $-2r = 0.0466(20)$.

[5] S.T. Chui, Phys. Rev. Lett. 48 (1982) 933; Phys. Rev. B 28 (1983) 178.
[6] Y. Saito, Phys. Rev. Lett. 48 (1982) 1114; Phys. Rev. B 26 (1982) 6239.
[7] A.Z. Patashinskii, private communication to H.H.
[8] F.R. Brown, T.J. Woch, Phys. Rev. Lett. 58 (1987) 2394.
[9] M. Creutz, Phys. Rev. D 36 (1987) 515.
[10] R.H. Swendsen, J.S. Wang, Phys. Rev. Lett. 58 (1987) 86.
[11] U. Wolff, Phys. Rev. Lett. 62 (1989) 361.
[12] U. Wolff, Nucl. Phys. B 334 (1990) 581.
[13] R. Gupta, C.F. Baillie, Phys. Rev. B 45 (1991) 2883.
[14] W. Janke, K. Nather, Phys. Rev. B 48 (1993) 7419.
[15] U. Wolff, Nucl. Phys. B 332 (1989) 759.
[16] W. Janke, preprint KOMA-96-17, hep-lat/9609045.
[17] R. Kenna, A.C. Irving, Phys. Lett. B 351 (1995) 273; Nucl. Phys. B 485 (1997) 583.