Surface properties at the Kosterlitz-Thouless transition

Bertrand Berche  
Laboratoire de Physique des Matériaux,  
Université Henri Poincaré, Nancy 1,  
F-54506 Vandœuvre les Nancy Cedex, France  
October 26, 2018

Monte Carlo simulations of the two-dimensional \(XY\) model are performed in a square geometry with free and mixed fixed-free boundary conditions. Using a Schwarz-Christoffel conformal mapping, we deduce the exponent \(\eta\) of the order parameter correlation function and its surface equivalent \(\eta_\parallel\) at the Kosterlitz-Thouless transition temperature. The well known value \(\eta(T_{KT}) = 1/4\) is easily recovered even with systems of relatively small sizes, since the shape effects are encoded in the conformal mapping. The exponent associated to the surface correlations is similarly obtained \(\eta_\parallel(T_{KT}) \simeq 0.54\).

1 Introduction

The two-dimensional classical \(XY\) model exhibits a non standard behaviour. Long-range order of spins with continuous symmetries is indeed forbidden according to the Mermin-Wagner theorem \([1]\), and thus there is no spontaneous magnetisation at finite temperature. The transition is governed by unbinding of topological defects. The low-temperature regime was investigated by Berezinskii \([2]\) and the mechanism of unbinding of vortices was studied by Kosterlitz and Thouless \([3]\) using renormalization group methods. For reviews, see e.g. Refs. \([4, 5]\).

The notations are specified below: we consider a \(2d XY\)-model on a square lattice with two-components spin variables \(\vec{\phi}_w = (\cos \theta_w, \sin \theta_w)\) located at the sites \(w\) of a lattice \(\Lambda\) of linear extent \(L\). The spins interact through the usual nearest-neighbour ferromagnetic interaction

\[
-H/k_B T = K \sum_w \sum_\mu \vec{\phi}_w \cdot \vec{\phi}_{w+\hat{\mu}}, \tag{1}
\]

where \(K = J/k_BT\) and \(\hat{\mu}\) is a unit vector in the \(\mu\)-direction.

At low temperature, the system is partially ordered, apart from the existence of vortices, which appear in pairs in increasing number with increasing temperature. In the low-temperature limit, the effect of vortices can be neglected and the behaviour
is governed by spin-wave excitations, obtained after expanding the cosine. This harmonic approximation is justified, provided that the spin disorientation remains small, i.e. at sufficiently low temperature. Within this approximation, the quadratic energy in the Boltzmann factor leads to a Gaussian equilibrium distribution and the two-point correlation function becomes

\[ \langle \vec{\phi}_{w_1} \cdot \vec{\phi}_{w_2} \rangle \simeq |w_1 - w_2|^{-1/2\pi K}, \]

hence

\[ \eta(T) = k_B T / 2\pi J. \]

When the temperature increases, the influence of vortices becomes more prominent, producing a deviation from the linear spin-wave contribution in equation (3), but the order parameter correlation function still decays algebraically with an exponent \( \eta(T) \) which depends on the temperature. The existence of such a scale-invariant power-law decay of the correlation function is the signature of a continuous line of fixed points at low temperatures. In this paper we are interested in the end point of this critical line where the topological transition takes place: at the transition temperature \( T_{KT} \) (usually called Berezinskii-Kosterlitz-Thouless critical temperature), the pairs are broken and the system becomes completely disordered. This very peculiar topological transition is characterised by essential singularities when approaching the critical point from the high temperature phase, and at \( T_{KT} \) the correlation function exponent takes the value \( \eta(T_{KT}) = 1/4 \).

In order to recover this result, many numerical studies were performed in the last decade using Monte Carlo simulations (see e.g. Refs. [7, 8, 9, 11, 12]), but the analysis was made difficult by the existence of logarithmic corrections, e.g.

\[ \langle \vec{\phi}_{w_1} \cdot \vec{\phi}_{w_2} \rangle \sim |w_{12}|^{-\eta \ln |w_{12}|} \],

at \( T_{KT} \). Due to these logarithmic corrections which make the fits quite difficult, the value of \( \eta \) at \( T_{KT} \) was a bit controversial as shown in table 1 of reference [12]. The resort to large-scale simulations, up to systems as large as \( L = 1200 \), was then needed in order to confirm this picture.

Recently, we proposed a rather different approach [13] which is easily implemented. We use the covariance law of correlation functions under the mapping of a two-dimensional system confined inside a square onto the half-infinite plane. The scaling dimensions are then obtained through a simple power-law fit when the correlators are expressed as functions of conveniently rescaled variables. The shape effects are explicitly encoded in the conformal mapping. This is the crucial point, since then even very small systems lead to promising results. We may then determine accurately the bulk correlation function exponent \( \eta \) at \( T_{KT} \) but also, by choosing convenient boundary conditions, the surface critical exponent which describes the decay of the correlation function parallel to a free surface, \( \eta_\parallel \).

2 Critical system confined inside a square with open boundaries

For a scale-invariant system at its critical point (which also exhibits the properties of isotropic scaling and short-range interactions), conformal invariance enable to include explicitly the shape dependence in the functional expression of the correlators
through the conformal covariance transformation under a mapping \( w(z) \):

\[
\langle \vec{\phi}_{w_1} \cdot \vec{\phi}_{w_2} \rangle = |w'(z_1)|^{-x} |w'(z_2)|^{-x} \langle \vec{\phi}_{z_1} \cdot \vec{\phi}_{z_2} \rangle.
\]

The functional expression of the correlation function inside the square geometry simply follows the mapping \( w(z) \) which realizes the conformal transformation of the half-plane \( z = x + iy \) \((0 \leq y < \infty)\) inside a square \( w = u + iv \) of size \( L \times L \) \((-L/2 \leq u \leq L/2, 0 \leq v \leq L)\) with free boundary conditions along the four edges. This is realized by a Schwarz-Christoffel transformation \[13\]

\[
w(z) = \frac{L}{2K} F(z, k), \quad z = \text{sn} \left( \frac{2Kw}{L} \right).
\]

Here, \( F(z, k) \) is the elliptic integral of the first kind, \( \text{sn} \left( \frac{2Kw}{L} \right) \) the Jacobian elliptic sine, \( K = K(k) \) the complete elliptic integral of the first kind, and the modulus \( k \) depends on the aspect ratio of \( \Lambda \) and is here solution of \( K(k)/K(\sqrt{1-k^2}) = \frac{1}{2} \). Using the mapping \[13\], one obtains the local rescaling factor in equation \( \ref{eq:rescaling_factor} \), \( w'(z) = \frac{L}{2K} \left( 1 - z^2 \right)^{-1/2} \). One simply has now to include in equation \( \ref{eq:rescaling_factor} \) the expected behaviour of \( \langle \vec{\phi}_{z_1} \cdot \vec{\phi}_{z_2} \rangle \) in the half-infinite geometry in order to get the functional expression of the corresponding quantity in the confined system. For example in the semi-infinite geometry \( z = x + iy \) (the free surface being defined by the \( x \) axis), the two-point correlation function is fixed up to an unknown scaling function: fixing one point \( z_1 \) close to the free surface \((z_1 = i)\) of the half-infinite plane, and leaving the second point \( z_2 \) explore the rest of the lattice, the following behaviour is expected:

\[
\langle \vec{\phi}_{z_1} \cdot \vec{\phi}_{z_2} \rangle \sim (y_1 - y_2)^{-x} \psi(\omega),
\]

with \( \eta = 2x \sigma \). The dependence on \( \omega = \frac{\sqrt{y_1^2 - y_2^2}}{y_1} \) of the universal scaling function \( \psi(\omega) \) is constrained by the special conformal transformation \[13\], and its asymptotic behaviour is implied by scaling e.g. \( \psi(\omega) \sim \omega^{x_2} \) when \( y_2 > 1, \) with \( x_2 = \frac{4}{\eta} \) the surface scaling dimension. Keeping \( w_1 \) fixed inside the square, the two-point correlation function becomes

\[
\langle \vec{\phi}_{w_1} \cdot \vec{\phi}_{w} \rangle_f \sim \left[ \kappa(w) \right]^{-x} \psi(\omega)
\]

\[
\kappa(w) = \text{Im} \left( \text{sn} \left( \frac{2Kw}{L} \right) \times \left( 1 - \text{sn}^2 \frac{2Kw}{L} \right) \left( 1 - k^2 \text{sn}^2 \frac{2Kw}{L} \right) \right)^{-1/2},
\]

where \( f \) specifies that the boundary conditions (BCs) are chosen free along the edges of the square. This expression is correct up to a constant amplitude determined by \( \kappa(w_1) \) which is kept fixed, but the function \( \psi(\omega) \) is still varying with the location of the second point, \( w \). This makes this expression not so useful in practice (see e.g. reference \[14\] for an application). In order to cancel the role of the unknown scaling function, it is more convenient to work with a density profile \( m(w) \) in the presence of symmetry breaking surface fields \( h_{\partial \Lambda} \) on some parts of the boundary \( \partial \Lambda \) of the lattice \( \Lambda \). In the case of fixed-free BCs denoted by \( +f \) (the spins located on the \( x > 0 \) half axis are kept fixed while those of the \( x < 0 \) are free), Burkhardt and Xue have shown in the case of Ising and Potts models that in the half-plane the order parameter profile obeys the following expression \[18\]:

\[
m_{+f}(z) = y^{-\eta/2} (\cos \frac{1}{2} \theta)^{\eta/2}.
\]

\[3\]
In the square geometry, the fixed-free BCs correspond to keeping the spins fixed for $u > 0$, and the corresponding profile is expected to obey the following ansatz:

$$m_{+f}(w) \sim \left( \frac{L}{2K} \right)^{-x_\sigma} [\kappa(w)]^{-x_\sigma} [\mu(w)]^{x_\mu} = \frac{1}{\sqrt{2}} \left( 1 + \text{Re} \left[ \frac{2Kw}{L} \right] \right)^{1/2}$$

where $\kappa(w)$ was defined in equation (8).

In this paper we will essentially apply equation (10) in order to determine the critical exponents $\eta$ and $\eta_\parallel$ at the KT point.

In Ref. [13], the bulk exponent was deduced from a similar analysis of the order parameter profiles in a square-shaped system with fully fixed BCs.

### 3 Monte Carlo simulations

The application of the simple power-law in equation (10) requires a relatively precise numerical determination of the order parameter profile of the 2$d$ XY model confined inside a square with mixed fixed-free boundary conditions. Fixing the spins along some part $\partial \Lambda$ of the boundary, e.g. $\vec{\phi}_w = (1,0), \forall w \in \partial \Lambda$, plays the role of ordering surface fields $\vec{h}_{\partial \Lambda(w)}$. The resort to cluster update algorithms (Wolff algorithm here) is necessary in order to prevent the critical slowing down: the central idea is the identification of clusters of sites using bond variables connected to the spin configuration. The spins of the clusters are then updated and the algorithm is particularly efficient if the percolation threshold of the bond process occurs at the transition temperature of the spin model. This ensures the updating of clusters of all sizes in a single MC sweep. For the XY model, Ising variables defined in the Wolff algorithm by the sign of the projection of the spin variables along some random direction. The bonds are then introduced through the Kasteleyn-Fortuin random graph representation. The percolation threshold for these bonds coincides with the Kosterlitz-Thouless point [20], which guarantees the efficiency of the Wolff cluster updating scheme [3] at $T_{KT}$. When one uses particular boundary conditions, with fixed spins along some surface as required here, the Wolff algorithm should become less efficient, since close to criticality the unique cluster will often reach the boundary and no update is made in this case. To prevent this, we use the symmetry properties of the Hamiltonian (1): even when the cluster reaches the fixed boundaries, it is updated, and the order parameter profile is then measured with respect to the new direction of the boundary spins, $m(w) = \langle \vec{\phi}_w \cdot \vec{\phi}_{\partial \Lambda} \rangle_{sq}$. The new configuration reached has the right statistical weight.

Using this procedure, we discard $10^6$ sweeps for thermalization, and the measurements are performed on $10^6$ production sweeps. The simulations at $T_{KT}$ on a typical system of size 100 $\times$ 100 takes a few hours on a standard PC with 733 MHz processor, to get a smooth profile as shown in figure 1.
4 Scaling of the order parameter profile \( m_{+f}(w) \)

In Ref. [13], we have shown that the logarithmic corrections at the KT point are negligible for the order parameter profile with fixed BCs. Assuming that there will be no substantial difference for fixed-free BCs, we perform a fit of \( \ln m_{+f}(w) \) against the two-dimensional linear expression, \( \text{const} - x_\sigma \ln \kappa(w) + x_1 \ln \mu(w) \), as expected from equation (10). The value obtained for the bulk correlation function exponent \( \eta \) will be a test for the absence of logarithmic corrections. The simulations are performed at the value \( k_B T_{KT}/J \approx 0.893 \) found in the literature, e.g. in Ref. [9]. The fit leads to accurate determinations of both exponents for different system sizes ranging between \( L = 20 \) and \( L = 200 \). Although it would easily be possible to produce simulations for larger systems, there is no need here, since the results are already quite stable as shown in table 1 and in figure 2.

This is fully coherent with the result of Kosterlitz and Thouless RG analysis \( \eta = 2x_\sigma = 1/4 \). We can thus also consider as reliable the value of the surface exponent \( \eta \parallel = 2x_1 \approx 0.54 \).

| \( L \) | \( x_\sigma \) | \( x_1 \) | \( \chi^2/d.o.f. \) |
|-------|-------|-------|-----------------|
| 20    | 0.149(33) | 0.290(15) | 0.691 \times 10^{-3} |
| 24    | 0.147(34) | 0.287(15) | 0.719 \times 10^{-3} |
| 28    | 0.134(22) | 0.280(12) | 1.210 \times 10^{-3} |
| 36    | 0.133(35) | 0.278(12) | 1.010 \times 10^{-3} |
| 48    | 0.133(35) | 0.279(10) | 0.743 \times 10^{-3} |
| 64    | 0.131(35) | 0.278(10) | 0.664 \times 10^{-3} |
| 100   | 0.126(17) | 0.275(14) | 0.544 \times 10^{-3} |
| 200   | 0.125(23) | 0.271(11) | 0.392 \times 10^{-3} |

Table 1:
Bulk and surface scaling dimensions of the order parameter at the Kosterlitz-Thouless transition. The values that we quote are those which correspond to a fit over all the lattice points (except those exactly at the boundaries) ignoring possible lattice effects.

Figure 1: MC simulations of the 2d XY model inside a square 48 \times 48 spins with mixed fixed-free boundary conditions at the KT transition temperature \( k_B T_{KT}/J = 0.893 \) (average over \( 10^6 \) MCS/spin after cancellation of \( 10^6 \) for thermalization).

Figure 2: Size dependence of the bulk and surface scaling dimensions at the KT transition plotted as a function of the inverse linear size of the lattice.
5 Scaling of the correlation function $\langle \vec{\phi}_{w_1} \cdot \vec{\phi}_{w} \rangle_f$ with free boundary conditions

Equation (8) provides a test in order to control the quality of the surface exponent obtained above. Indeed, if one plots $\langle \vec{\phi}_{w_1} \cdot \vec{\phi}_{w} \rangle_{sq} \times \left[ \kappa(w) \right]^{x_\sigma} \times \omega$, one should obtain the universal scaling function $\psi(\omega)$ whose asymptotic large distance behaviour should lead to a consistent surface exponent through the expected power-law behaviour $\omega^{x_\sigma}$.

Figure 3: Universal scaling function of the surface-volume correlation function for $L = 100$. The power-law behaviour $\psi(\omega) \sim \omega^{x_\sigma}$ shown in dotted line agrees with a value $x_\sigma \approx 0.277$.

The scaling function $\psi(\omega)$ is shown in figure 3. It exhibits a clear power-law behaviour consistent with the previous value of the surface scaling dimension.

We mention here that the data were obtained for both quantities, $\langle \vec{\phi}_{w_1} \cdot \vec{\phi}_{w} \rangle_f$ and $m_+f(w)$, with completely independent runs, since the boundary conditions are different in equations (8) and (10) and the quantities themselves are different (2-point or 1-point correlators). The data collapse is quite good and supports the validity of equation (8).

6 Conclusion

In this paper we have performed standard MC simulations of the 2d XY model at the Kosterlitz-Thouless topological transition. Combined to the use of a conformal mapping, they provide a simple numerical determination of bulk and surface critical exponents associated to the algebraic decay of the correlation function. The well known result of Kosterlitz and Thouless for the bulk exponent is recovered and as far as the author knows this is the first determination of the surface exponent $\eta_\parallel \approx 0.54$. On the contrary to the bulk case, $\eta_\parallel$ is different from the Ising value (which is equal to $\eta_\parallel^{Ising} = 1$) [21].

References

[1] N.D. Mermin and H. Wagner, Phys. Rev. Lett. 22 (1966) 1133; P.C. Hohenberg, Phys. Rev. 158 (1967) 383.

[2] V.L. Berezinskii, Sov. Phys. JETP 32 (1971) 493.

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

[4] J.M. Kosterlitz and D.J. Thouless, Prog. Low Temp. Phys 78 (1978) 371; D.R. Nelson, in Phase Transitions and
Critical Phenomena, ed. by C. Domb and J.L. Lebowitz, Academic Press, London 1983, p. 1.

[5] C. Itzykson and J.M. Drouffe, Statistical field theory, Cambridge University Press, Cambridge 1989, vol. 1.

[6] F. Wegner, Z. Phys. 206 (1967) 465; G. Sarma, Solid State Comm. 10 (1972) 1049.

[7] J.F. Fernández, M.F. Ferreira and J. Stankiewicz, Phys. Rev. B 34 (1986) 292; R. Gupta, J. DeLapp, G.G. Batrouni, G.C. Fox, C.F. Baillie and J. Apostolakis, Phys. Rev. Lett. 61 (1988) 1996; L. Bifferale and R. Petronzio, Nucl. Phys. B 328 (1989) 677.

[8] U. Wolff, Nucl. Phys. B 322 (1989) 759.

[9] R. Gupta and C.F. Baillie, Phys. Rev. B 45 (1992) 2883.

[10] W. Janke and K. Nather, Phys. Rev. B 48 (1993) 7419; P. Olsson, Phys. Rev. B 52 (1995) 4526.

[11] W. Janke, Phys. Rev. B 55 (1997) 3580.

[12] R. Kenna and A.C. Irving, Nucl. Phys. B 485 [FS] (1997) 583.

[13] B. Berche, A.I. Fariñas Sanchez and R. Paredes, e-print [cond-mat/0208521].

[14] M. Henkel, Conformal Invariance and Critical Phenomena, Springer, Heidelberg 1999.

[15] M. Lavrentiev and B. Chabat, Méthodes de la théorie des fonctions d’une variable complexe, Mir, Moscou 1972, Chap. VII.

[16] J. L. Cardy, Nucl. Phys. B 240 [FS12] (1984) 514.

[17] C. Chatelain and B. Berche, Phys. Rev. E 60 (1999) 3853.

[18] T.W. Burkhardt and T. Xue, Phys. Rev. Lett. 66 (1991) 895; T.W. Burkhardt and T. Xue, Nucl. Phys. B354 (1991) 653.

[19] Burkhard and Xue gave several predictions for conformally invariant profiles in strip geometries $k + il$ or in their half-infinite counterpart $z = x + iy$: considering a semi-infinite system described by $z = x + iy = \rho e^{i\theta}$, $y \geq 0$, ordinary scaling implies a functional form in the half-plane, $m_{ab}(z) = y^{-x_s} F_{ab}(x/\rho)$, where $ab$ specifies the boundary conditions. Under the logarithmic transformation into a strip of width $L$, $L \ln z = k + il$, one obtains the order parameter profile as $m_{ab}(l) = \left[ L \pi \sin \left( \frac{\pi l}{L} \right) \right]^{-x_s} F_{ab} \left( \frac{\pi l}{L} \right)$.

[20] I. Dukovski, J. Machta and L.V. Chayes, Phys. Rev. E 65 (2002) 026702.

[21] K. Binder, in Phase Transitions and Critical Phenomena, edited by C. Domb and J.L. Lebowitz (Academic Press, London, 1983), Vol. 8, p. 1.