Kosterlitz-Thouless transition of thin films in the 3D XY universality class

Martin Hasenbusch

ITP, Universität Leipzig

Leipzig, 27 November 2008

Outline of the talk

- The 2-component ϕ^4 model; thin film geometry
- Phenomenological couplings (Binder cumulant etc.)
- Solid on Solid (SOS) models; Sine-Gordon model
- The RG-flow
- Finite size scaling at the KT-transition
- The KT-transition temperature of thin films

Talk is based on:

M. H., The two dimensional XY model at the transition temperature: A high precision Monte Carlo study, cond-mat/0502556, J. Phys. A: Math. Gen. 38 (2005) 5869.

M. H., The Binder Cumulant at the Kosterlitz-Thouless Transition , arXiv:0804.1880 [cond-mat], J. Stat. Mech. (2008) P08003.

M. H., Kosterlitz-Thouless transition in thin films: A Monte Carlo study of three-dimensional lattice models, arXiv:0811.2178

Motivation:

Comparison with experiments on thin films of ^{4}He

λ-transition of ^{4}He shares three-dimensional XY universality class

Simple cubic lattice sites $x = (x_0, x_1, x_2)$; $1 \leq x_i \leq L_i$

ϕ^4 model:

$$H_{\phi^4} = -\beta \sum_{<x,y>} \vec{\phi}_x \cdot \vec{\phi}_y + \sum_x \left[\vec{\phi}_x^2 + \lambda(\vec{\phi}_x^2 - 1)^2\right]$$

$\vec{\phi} \in \mathbb{R}^2$ $< xy >$ pair of nearest neighbours

Boltzmann factor: $\exp(-H_{\phi^4})$

$\lambda \to \infty$: $|\vec{\phi}| = 1$ $\Longrightarrow$ XY model $\lambda = 0$: Gaussian model

$$\xi = f(\lambda)\ t^{-\nu}\ \ (1 + a(\lambda)t^{\Delta} + b(\lambda)t + ...)\ \ ; \quad \Delta \approx 0.5$$

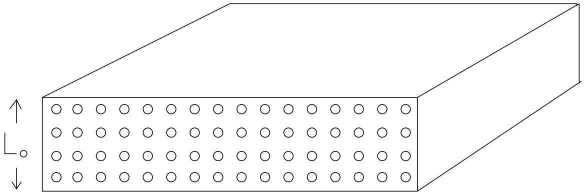
There exists λ^* such that $a(\lambda^*) = 0$; Campostrini et al. $\lambda^* = 2.15(5)$

Thin films

Experiment: The order parameter vanishes at the boundary

$\Longrightarrow$

lattice model: Free boundary conditions in the short direction



Periodic boundary conditions in the other two directions

Dirichlet boundary conditions:

Additional corrections to scaling $\propto L_0^{-1}$: $L_{0,eff} = L_0 + L_s$

For $\xi_{bulk} \gg L_0$ effectively two-dimensional behaviour is expected

$\Longrightarrow$ Kosterlitz-Thouless (KT) transition

For $\xi_{bulk}, L_0 \gg 1$ physics is governed by L_0/ξ_{bulk}

In particular KT transition takes place at a universal value of L_0/ξ_{bulk}

It follows (M.E. Fisher 1971)

$$T_{c,3d} - T_{KT}(L_0) \simeq L_0^{-1/\nu}$$

Observables

The total magnetisation and the magnetic susceptibility

$$\vec{M} = \sum_x \vec{\phi}_x \qquad \chi = \frac{1}{L_0 L_1 L_2} \langle \vec{M}^2 \rangle$$

The Binder cumulant

$$U_4 = \frac{\langle (\vec{M}^2)^2 \rangle}{\langle \vec{M}^2 \rangle^2}$$

The Second moment correlation length

$$\xi_{2nd,1} = \sqrt{\frac{\chi/F_1 - 1}{4 \sin(\pi/L_1)^2}} \qquad F_1 = \frac{1}{L_0 L_1 L_2} \left\langle \left| \sum_x \exp\left(i \frac{2\pi x_1}{L_1} \right) \vec{\phi}_x \right|^2 \right\rangle$$

helicity modulus Υ

Rotated boundary conditions in one direction:
For $x_1 = L_1$ and $y_1 = 1$ the term $\vec{\phi}_x \vec{\phi}_y$ in the Hamiltonian is replaced by

$$\vec{\phi}_x \cdot R_\alpha \vec{\phi}_y =$$

$$\phi_x^{(1)} \left(\cos(\alpha)\phi_y^{(1)} + \sin(\alpha)\phi_y^{(2)}\right) + \phi_x^{(2)} \left(-\sin(\alpha)\phi_y^{(1)} + \cos(\alpha)\phi_y^{(2)}\right)$$

The helicity modulus is then given by

$$\Upsilon = \frac{L_1}{L_0 L_2} \frac{\partial^2 \log Z(\alpha)}{\partial \alpha^2}\bigg|_{\alpha=0}$$

Note that $L_0 \Upsilon$ is dimensionless

Ratio of partition functions Z_a/Z_p

a: anti-periodic boundary conditions in one direction and periodic (or free) in the others

p: all periodic or free

Can be measured with the boundary flip cluster algorithm

Dimensionless quantities also called phenomenological couplings: U_4, ξ_{2nd}/L, and Z_a/Z_p; in 2D also Υ.

Second order phase transition: (Binder Crossing)

$$R = R^* + c(\beta - \beta_c)L^{1/\nu} + dL^{-\omega} +$$

Two-dimensional Solid-on-Solid models

Two-dimensional XY models on a square lattice are exactly related by duality with Solid-on-Solid (SOS) models
See R. Savit, Rev. Mod. Phys. 52 (1980) 453
Absolute value SOS model

$$H_{ASOS} = \tilde{\beta}_{ASOS} \sum_{<x,y>} |h_x - h_y|$$

Discrete Gaussian SOS model (dual of the Villian model)

$$H_{DGSOS} = \frac{\tilde{\beta}_{DGSOS}}{2} \sum_{<x,y>} (h_x - h_y)^2$$

where h_x is integer. In general: $H_{SOS} = \sum_{<x,y>} V(|h_x - h_y|)$

The Boltzmann factor of an 2D XY model: $(\vec{s}_x \vec{s}_y) = \cos(\theta_{<xy>})$

$$B(\{\vec{s}\}) = \prod_{<xy>} w(\theta_{<xy>})$$

The Boltzmann factor of an SOS model:

$$\tilde{B}(\{h\}) = \prod_{<xy>} \tilde{w}(|h_x - h_y|)$$

The weight functions of dual models are related as

$$w(\theta) = \sum_{n=-\infty}^{\infty} \tilde{w}(n) \cos(n\theta)$$

$$\tilde{w}(n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{d}\theta \; w(\theta) \cos(n\theta) \; .$$

BCSOS model equivalent to six-vertex model (van Beijeren 1977)

$$H_{BCSOS} = \beta_{BCSOS} \sum_{[x,y]} |h_x - h_y|$$

$[x, y]$ pair of next to nearest neighbours.
Constraint $|h_x - h_y| = 1$ for nearest neighbours.

$$\xi \simeq \frac{1}{4} \exp\left(\frac{\pi^2}{8\sqrt{\frac{1}{2}\ln 2}} t^{-1/2} \right) \qquad t = \frac{\beta - \beta_R}{\beta_R}$$

with $\beta_R = \frac{1}{2}\ln 2$ has the form predicted for the KT-transition

$\Rightarrow$ matching of SOS models with BCSOS model
M.Hasenbusch, M.Marcu and K.Pinn, Physica A 208 (1994) 124
M.Hasenbusch and K.Pinn, J.Phys.A 30 (1997) 63

Sine-Gordon model

$$S_{SG} = \frac{1}{2\beta} \sum_{x,\mu} (\phi_x - \phi_{x+\hat{\mu}})^2 - z \sum_x \cos(2\pi\phi_x)$$

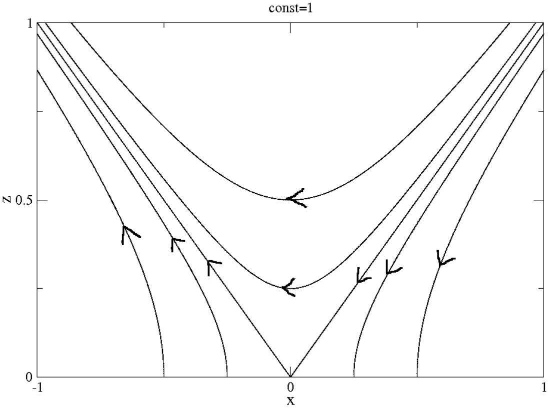
where $\phi \in \mathbb{R}$

RG-flow equations: ($x = \pi\beta - 2$)
See e.g. D.J. Amit, Y.Y. Goldschmidt and G. Grinstein, J. Phys. A 13 (1980) 585

$$\frac{\partial z}{\partial t} = -xz + \ldots \; , \qquad \frac{\partial x}{\partial t} = -const \;\; z^2 + \ldots \; ,$$

where $t = \ln l$ is the logarithm of the length scale l at which the couplings are taken

Solutions are characterized by $x^2 - const\ z^2 = a^2$



Flow at the transition: $x = \frac{1}{t+c} = \frac{1}{\ln l + C}$

Spinwave approximation

Gaussian Hamiltonian

$$H_{SW} = \frac{\beta_{SW}}{2} \sum_{x,\mu} (\theta_x - \theta_{x+\hat{\mu}})^2$$

where now

$$\vec{s}_x = (\cos(\theta_x), \sin(\theta_x))$$

Sine-Gordon at $z = 0$ and the spin-wave model are also related by duality: $\beta_{SG} = \beta_{SW}$.

Finite size scaling of phenomenological couplings R

For all quantities we are interested in:

$$R(\beta, z) = R_0(\beta) + O(z^2)$$

$\Rightarrow$ Compute $R(\beta)$ in spinwave approximation; Insert

$$\beta = \frac{2}{\pi} + \frac{\pi}{\ln L + C}$$

to get the behaviour at the KT transition temperature. For a lattice with periodic boundary conditions, isotropic couplings and size L^2

$$\Upsilon_{transition} = \frac{2}{\pi} + \frac{1}{\pi}\frac{1}{\ln L + C} + \ \ldots$$

H. Weber and P. Minnhagen, Phys. Rev. B 37 (1988) 5986

Note $2/\pi = 0.6366197722...$ Due to winding configurations M.H.2005

$$\Upsilon_{L^2,transition} = 0.63650817819... + \frac{0.318899454...}{\ln L + C} + \ ...$$

M.H. 2005:

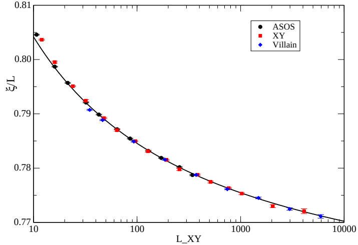
$$\left.\frac{\xi_{2nd}}{L}\right|_{L^2,transition} = 0.7506912... + \frac{0.212430...}{\ln L + C} + \ ... \ .$$

M.H. 2008b:

$$\left.\frac{Z_a}{Z_p}\right|_{L^2,transition} = 0.0864272337... - 0.135755793... \frac{1}{\ln L + C} + ...$$

M.H. 2008a:

$$U_{4,L^2,transition} = 1.018192(6) - \frac{0.017922(5)}{\ln L + C} + ...$$



Hasenbusch and Pinn 1997

Matching with BCSOS

$$\beta_{KT}^{XY} = 1.1199(1)$$

$$\beta_{KT}^{Villain} = 0.75154(23)$$

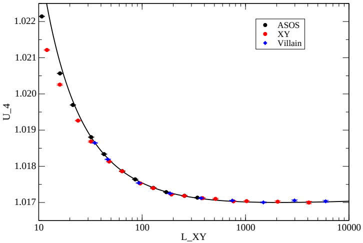
$$\tilde{\beta}_{KT}^{ASOS} = 0.80608(2)$$

and

$$b_m^{XY} = 0.93(1)$$

$$b_m^{Villain} = 0.32(1)$$

$$b_m^{ASOS} = 2.78(3)$$



e.g. $L_{XY} = L_{ASOS}\, b_m^{XY} / b_m^{ASOS}$

Statistics:

typically 10^7 measurements

$\tilde{\beta} = 0.80608 \quad :$

$$U_{4,ASOS}(L) = 1.018192 - \frac{0.017922}{\ln L - 1.18} + \frac{0.06769}{(\ln L - 1.18)^2}$$

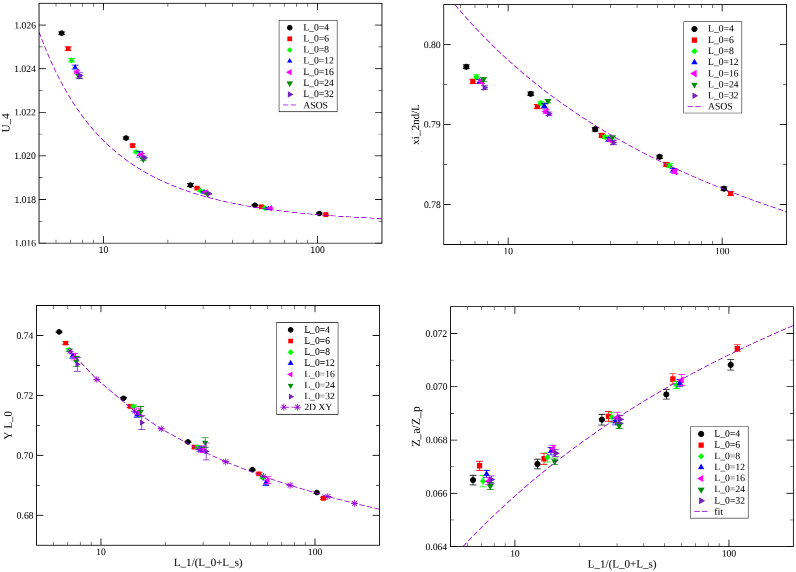
$$\frac{\xi_{2nd,ASOS}(L)}{L} = 0.7506912 + \frac{0.212430}{\ln L + 0.573}$$

Final results for the inverse of the KT transition temperature

L_0	β_{KT}
4	0.60968(1)[1]
6	0.56825(1)[1]
8	0.549278(5)[9]
12	0.532082(3)[5]
16	0.524450(2)[3]
24	0.517730(2)[2]
32	0.514810(1)[2]
∞	0.5091503(6)

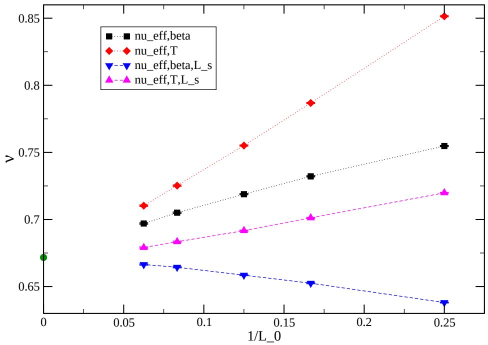
The matching factor $(L_0 + L_s) L_{ASOS}/L_1 = b_{ASOS,film} = 5.0(5)$

(L_1/L_0 up to 128 for $L_0 = 4, 6$; up to 32 for $L_0 = 32$)
Statistics: typically 2×10^6 measurements


U_4
1.026
1.024
1.022
1.020
1.018
1.016
10
100
L_0=4
L_0=6
L_0=8
L_0=12
L_0=16
L_0=24
L_0=32
ASOS
xi_2nd/L
0.80
0.79
0.78
ASOS
Y L_0
0.74
0.72
0.70
0.68
2D XY
L_1/(L_0+L_s)
Z_a/Z_p
0.072
0.070
0.068
0.066
0.064
fit

$$\nu_{eff,\beta}(L_0) = -\ln(2)/\ln\left(\frac{\beta_{KT}(2L_0) - \beta_{c,3d}}{\beta_{KT}(L_0) - \beta_{c,3d}}\right)$$

$$\nu_{eff,\beta,L_s}(L_0) = -\ln\left(\frac{2L_0 + L_s}{L_0 + L_s}\right) / \ln\left(\frac{\beta_{KT}(2L_0) - \beta_{c,3d}}{\beta_{KT}(L_0) - \beta_{c,3d}}\right)$$



$$\beta_{KT}(L_0) - \beta_{c,3D} = a(L_0 - L_s)^{-1/\nu} \quad \times (1 + c(L_0 - L_s)^{-1/\nu})$$

Fixing $\beta_c = 0.5091503$ and $\nu = 0.6717$

$L_{0,min}$	a	L_s	c	χ^2/d.o.f.
4	1.0321(11)	1.158(29)	1.38(11)	3.80
6	1.0286(13)	1.037(36)	0.90(13)	0.39
8	1.0284(18)	1.030(59)	0.87(23)	0.57

Summary

- We have determined the behaviour of various phenomenological couplings at the KT transition
- The behaviour of Υ, ξ_{2nd}/L, Z_a/Z_p is well described by the leading logarithmic correction
- This is quite different in the case of the Binder cumulant U_4: a term $\propto 1/(lnL)^2$ is needed to fit the data
- Using the behaviour of ξ_{2nd}/L and U_4 we determine the KT transition temperature of thin films with high precision.
- In order to fit the data for the KT transition temperature as a function of the thickness L_0, surface corrections $L_{0,eff} = L_0 + L_s$ and leading analytic corrections have to be included into the fit.

Acknowledgement:
This work is partially supported by DFG under grant No JA 483/23-1.