The Kosterlitz-Thouless transition in thin films: Monte Carlo simulations of 3D lattice models

Martin Hasenbusch

Institut für Physik, Humboldt-Universität zu Berlin

CompPhys13, 29 November 2013

Overview

- The Kosterlitz-Thouless transition
- 2D finite size scaling of Υ, ξ_{2nd}/L and U_4
- Numerical results for films, 3D finite size scaling
- Comparison with experiments on films of ^{4}He

2D XY-model on the square lattice

$$H = -\beta \sum_{<x,y>} \vec{s}_x \vec{s}_y$$

where the spin $\vec{s}_x$ is unit-vector with two real components.
$< xy >$ is a pair of nearest neighbour sites on the lattice.

Theorem of Mermin and Wagner (1966): No long range order

Spin-wave approximation: Gaussian approximation of the reduced Hamiltonian

$$H_{SW} = \frac{\beta_{SW}}{2} \sum_{<x,y>} (\phi_x - \phi_y)^2$$

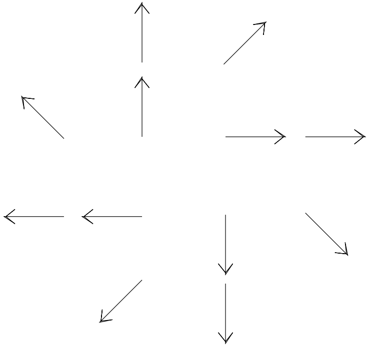
where $\vec{s}_x = (\cos\phi_x, \sin\phi_x)$. The two-point function behaves as

$$G(x-y) = \langle \vec{s}_x \vec{s}_y \rangle_{SW} \propto |x-y|^{-\eta}$$

with $\eta = \frac{1}{2\pi\beta_{SW}}$

Berezinskii (1971), Kosterlitz and Thouless (1973):

At sufficiently high temperatures vortices alter the physics



Energy of a vortex of radius R:

$$E_{vor} = \pi \int_1^R \mathrm{d}r \, \frac{1}{r}$$

$$= \pi \ln R$$

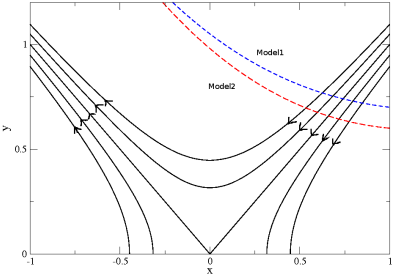
Analysis of the renormalization group (RG) flow

$x = \pi\beta_{SW} - 2 \quad ; \quad y$ (related with chemical potential for vortices)

The flow equations:

$$\frac{dx}{dl} = -y^2$$
$$\frac{dy}{dl} = -xy$$

where $l = \ln a$ is the logarithm of the cut-off scale. The solutions satisfy $x^2 - y^2 = const$



The correlation length in the high temperature phase

$$\xi \simeq a \exp(b t^{-1/2}) \quad , \quad t = \frac{\beta_{KT} - \beta}{\beta_{KT}}$$

The magnetic susceptibility in the high temperature phase

$$\chi \simeq \xi^{2-\eta}$$

with $\eta = 1/4$.

Singular part of free energy density

$$f_s \propto \xi^{-2} \propto \exp(-2 b t^{-1/2})$$

$\partial^n f_s / \partial t^n$ at $t = 0$ exits for any $n \Rightarrow$ KT-transition is of infinite order

BCSOS model (van Beijeren 1977): $H_{BSOS} = \beta_{BSOS} \sum_{[xy]} |h_x - h_y|$ where $[xy]$ is a pair of next-to-nearest neighbours. Constraint on nearest neighbours: $|h_x - h_y| = 1$.

Equivalent to the exactly solved F model (Lieb 1967)

$$\beta_{BSOS,KT} = \frac{1}{2}\ln 2 \quad ; \quad \xi \simeq \frac{1}{4}\exp\left(\frac{\pi^2}{8\sqrt{\frac{1}{2}\ln 2}}\left(\frac{\beta_{BSOS}-\beta_{BSOS,KT}}{\beta_{BSOS,KT}}\right)^{-\frac{1}{2}}\right)$$

Numerical matching of SOS models with the BCSOS at the KT-transition, Hasenbusch and Pinn (1997)

$$\begin{aligned} \beta_{XY,KT} &= 1.1199(1) & b_{XY,BCSOS} &= L_{XY}/L_{BCSOS} = 0.93(1) \\ \beta_{DG,KT} &= 0.6653(2) & b_{DG,BCSOS} &= 0.32(1) \\ \beta_{ASOS,KT} &= 0.80608(2) & b_{ASOS,BCSOS} &= 2.78(3) \end{aligned}$$

Finite size scaling at the KT-transition

- Compute dimensionless quantities Υ, Z_a/Z_p, ξ/L, U_4, ... in spin-wave approximation

- Put in $\beta_{sw} = \frac{2}{\pi} + \frac{1}{\pi}\frac{1}{\ln L + C}$ where we identify the lattice size L as the relevant length scale

Vicari, Pelisetto, Phys.Rev. E87 (2013) 3, 032105

$\beta_{sw} = \frac{2}{\pi} + \frac{1}{\pi}\frac{1}{\ln L/l_0 + \frac{1}{2}\ln\ln L/l_0}$

-Note that for periodic boundary conditions y enters the observables only at $O(y^2)$. Error $O((\ln L/l_0)^{-2})$

Lattice of the size L^2 with periodic boundary conditions:

Well known behaviour of the helicity modulus

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

(Note $2/\pi = 0.63661977236...$)

(M.H. 2005): Second moment correlation length

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

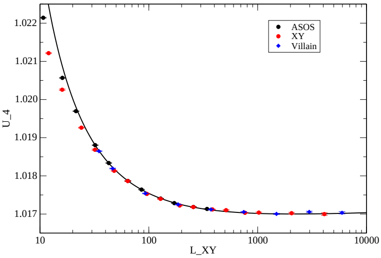
(M.H. 2008): Binder cumulant $U_4 =< (\vec{m}^2)^2 > / < \vec{m}^2 >^2$

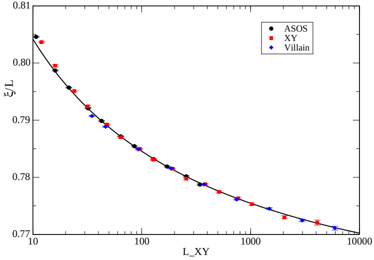
$$U_{4,L^2,transition} = 1.018192(6) - \frac{0.017922(5)}{\ln L + C} + ... \, ,$$

Dual of ASOS model at $\tilde{\beta} = 0.80608$ and $L_{min} = 96$: (M.H. 2008)

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

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





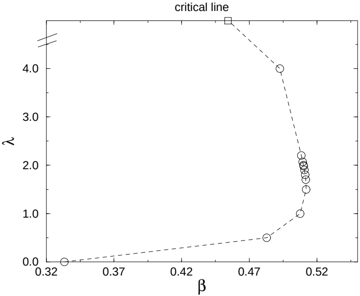
2-component ϕ^4 model:

$$H = -\beta \sum_{x,\mu} \vec{\phi}_x \vec{\phi}_{x+\hat{\mu}} + \sum_x \left[\vec{\phi}_x^2 + \lambda(\vec{\phi}_x^2 - 1)^2\right]$$

where the field variable $\vec{\phi}_x$ is a vector with 2 real components.
x is a site on a simple cubic lattice and $\hat{\mu}$ a unit vector in μ direction.

The partition function is given by

$$Z = \left[\prod_x \prod_{i=1}^{2} \int d\phi_x^{(i)}\right] \exp(-H)$$



The correlation length behaves as

$$\xi = \xi_{0,\pm}(\lambda)\,|t|^{-\nu}\;\;(1 + c(\lambda)t^{\theta} + ...)$$

where $t = \beta_c - \beta$ is the reduced temperature, $\nu = 0.6717(1)$ (Campostrini et al. 2006) is the exponent of the correlation length and $\theta = \nu\omega \approx 0.5$ the exponent of the leading correction. The helicity modulus $\Upsilon = 1/\xi_T$ is defined in the low temperature phase. ξ_T is the transversal correlation length.

$$\lim_{t\to 0} \xi_{2nd}(t)\Upsilon(-t) = 0.411(2)$$

The improved model: $c(\lambda^*) = 0$ (Idea: Chen, Fisher, Nickel 1982)
Numerically (Campostrini et al. 2006): $\lambda^* = 2.15(5)$

Here we study $\lambda = 2.1$:

$$\beta_c = 0.5091503(6) \qquad \xi_{0,+} = 0.26362(8) \qquad \left|\frac{c(2.1)}{c(XY)}\right| \lesssim \frac{1}{30}$$

Film geometry:

System is finite in one direction and infinite in the other two

In our simulations: $L_0 \ll L_1 = L_2$

free boundary conditions: relevant for films of ^{4}He in the neighbourhood of the λ-transition

Corrections $\propto L_0^{-1}$ (Capehart and Fisher 1976, Diehl, Dietrich and Eisenriegler 1983); Can be cast into the form $L_{0,eff} = L_0 + L_s$. For our model $L_s = 1.02(7)$.

Results of the matching:

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)

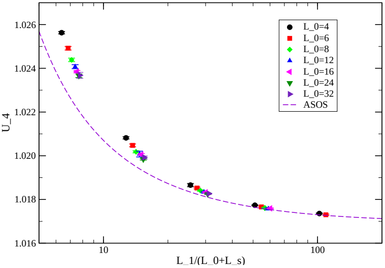
$$b_{ASOS,film} = L_{ASOS}(L_0 + L_s)/L$$

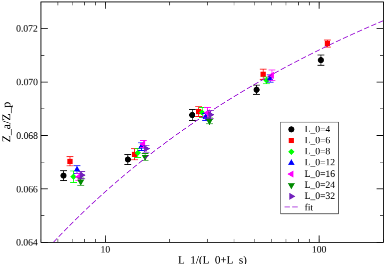
$$= 5.0(5)$$

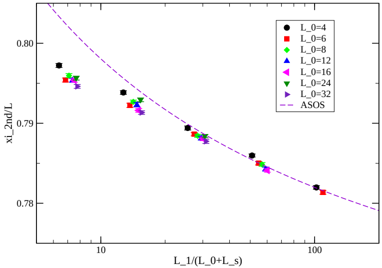
Ansatz (motivated by Fisher 1971)

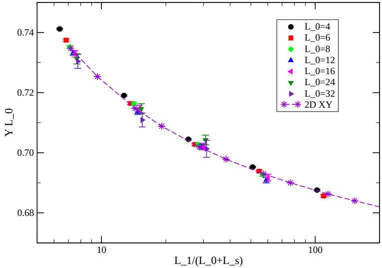
$$\beta_{KT}(L_0) - \beta_{c,3D} = a[L_0 + L_s]^{-1/\nu} \times (1 + c[L_0 + L_s]^{-1/\nu})$$

$L_{0,min}$	a	L_s	c	χ^2/DOF
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


U_4
1.026
1.024
1.022
1.020
1.018
1.016
10
100
L_1/(L_0+L_s)
L_0=4
L_0=6
L_0=8
L_0=12
L_0=16
L_0=24
L_0=32
ASOS


Z_a/Z_p
0.072
0.070
0.068
0.066
0.064
10
100
L 1/(L 0+L s)
L_0=4
L_0=6
L_0=8
L_0=12
L_0=16
L_0=24
L_0=32
fit


xi_2nd/L
0.80
0.79
0.78
10
100
L_1/(L_0+L_s)
L_0=4
L_0=6
L_0=8
L_0=12
L_0=16
L_0=24
L_0=32
ASOS


Y L_0
0.74
0.72
0.70
0.68
10
100
L_1/(L_0+L_s)
L_0=4
L_0=6
L_0=8
L_0=12
L_0=16
L_0=24
L_0=32
2D XY

Comparison of our result $L_{0,KT}/\xi_\perp = 1.595(7)$ with experimental results for films of ^{4}He, $T_\lambda \approx 2.17$ K

Sabisky and Anderson, Phys. Rev. Lett. **30** 1122, (1973)
KT-thickness determined by the onset of superfluidity.
Using films on a CaF_2 substrate of a thickness up to $\approx 80\AA$ they find

$$L_{0,KT} = 5.1(1-T/T_\lambda)^{-2/3}\AA \quad ; \quad \Upsilon L_{0,KT} \approx 1.545$$

van de Laar, van der Hoek and van Beelen, Physica B **216** 24, (1995) have studied films of a thickness up to $47\AA$ with glass as substrate. They quote the final result

$$L_{0,KT} = 0.43\AA + 1.61\xi_\perp$$

Note that more recent experiment by Gasparini et al. with thicker films match less well.

Conclusions:

- Properties of the KT-transition theoretically well established
- At the KT-transition: Logarithmic corrections have to be taken into account in a Monte Carlo study: Exact results for FSS of Υ , ξ_{2nd}/L , and U_4
- We have accurately determined the transition temperature of thin films in the 3D XY universality class We confilm the KT-nature of the transition
- The KT-temperature scales as predicted by 3D finite size scaling (Fisher 1971, Barber 1983)
- Corrections $\propto L_0^{-1}$ can be described by replacing L_0 by $L_{0,eff} = L_0 + L_s$
- Our result $L_{0,KT}/\xi_\perp = 1.595(7)$ is nicely consistent with that for thin films of ^{4} He

M. Hasenbusch,
Kosterlitz-Thouless transition in thin films: A Monte Carlo study of three-dimensional lattice models
arXiv:0811.2178 [cond-mat], J. Stat. Mech. (2009) P02005
and refs. therein

I like to thank W Janke for support. The project was funded by the DFG under grant No. JA 483/23-1.