Phase transition of films in the Ising universality class

Martin Hasenbusch

Institut für Physik, Humboldt-Universität zu Berlin

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Overview

- Blume-Capel and Ising model on the simple cubic lattice, Film geometry
- The two-dimensional Ising model, Finite size scaling
- Numerical results
- Universal amplitude ratios

Reduced Hamiltonian of the Ising model on the simple cubic lattice

$$H = -\beta \sum_{<x,y>} s_x s_y - h \sum_x s_x$$

Lattice sites: $x = (x_0, x_1, x_2)$ with $x_i \in \{1, 2, ..., L_i\}$
Spin $s_x \in \{-1, 1\}$, pair of nearest neighbours $< xy >$

Films: $L_0 \gg L_1, L_2$, periodic boundary conditions in 1-, and 2-directions. Periodic or free boundary conditions in 0-direction. These boundary conditions do not break the $\mathbb{Z}_2$ symmetry.

Blume-Capel model: $s_x \in \{-1, 0, 1\}$

$$H = -\beta \sum_{<x,y>} s_x s_y + D \sum_x s_x^2 - h \sum_x s_x$$

For $D = 0.656(20)$ leading corrections to scaling vanish. We simulate at $D = 0.655$ since β_c and the values of various amplitudes are accurately known.

(1) Films undergo a phase transition. If continuous, in the universality class of the two-dimensional Ising model (Svetitsky-Yaffe conjecture in the case gauge models.)

(2) Based on standard RG-arguments one expects (Fisher 1971, Capehart and Fisher 1976)

$$\beta_{c,2D}(L_0) - \beta_{c,3D} \simeq a L_0^{-1/\nu}$$

where $\nu = 0.63002(10)$ is the critical exponent of the correlation length of the 3D bulk system.

We are aiming at:

- compute $\beta_{c,2D}(L_0)$ accurately for a range of thicknesses L_0.
- check (1) and (2)

2D Ising model

on the square lattice is exactly solved for $h = 0$: Onsager, Kaufman, Yang, Wu, Baxter ..., accurate numerical results also for $h \neq 0$

$$\beta_c = \frac{1}{2} \ln(1+\sqrt{2}) = 0.440686793...$$

The correlation length in the thermodynamic limit

$$\xi \simeq \xi_{0,\pm} |\tau|^{-\nu_{2D}}$$

where

$$\tau = \frac{1}{2}\left(\frac{1}{\sinh 2\beta} - \sinh 2\beta\right)$$

and $\nu_{2D} = 1$, $\xi_{0,+} = 1/\sqrt{2}$ and $\xi_{0,-} = \xi_{0,+}/2$.

Important for our purpose: dimensionless, RG-invariant quantities on finite lattices: For $L_1 = L_2 = L$, (anti)-periodic boundary conditions

$$R_Z^* = 0.372884880824589...$$

where $R_Z = \frac{Z_a}{Z_p}$ and $R^* := \lim_{L\to\infty} R(L, \beta_c)$

$$\lim_{L\to\infty} [\bar{S}/L]_{2DIsing} = \lim_{L\to\infty} \frac{1}{L} \left. \frac{\partial Z_a/Z_p}{\partial \tau} \right|_{\tau=0} = 0.3021247100407...$$

Binder Cumulant (J. Salas and A. D. Sokal, 1999)

$$U_4^* = 1.1679229 \pm 0.0000047$$

Second moment correlation length over lattice size

$$(\xi_{2nd}/L)^* = 0.9050488292 \pm 0.0000000004$$

Variant of the Binder crossing: Estimate $\bar{\beta}_{c,2D}(L_0, L)$ of $\beta_c(L_0)$ is obtained by solving

$$R(\beta, L_0, L) = R^*$$

with respect to β. Convergence:

$$\bar{\beta}_{c,2D}(L_0, L) - \beta_{c,2D}(L_0) = c(L_0) L^{-1/\nu_{2D}-\omega} + \ldots$$

where $\omega = 2$ due to the breaking of rotational invariance by the lattice. However $\omega_{eff} = 7/4$ for U_4 and ξ_{2nd}/L due to the analytic background in the magnetic susceptibility.

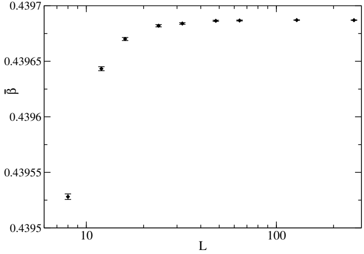
$\Longrightarrow$ R_Z optimal quantity (M. Caselle, M. H. 1996)

Can be computed in MC simulations by using the boundary flip algorithm; M.H. (1993)

free boundary conditions

H. Kitatani, M. Ohta, and N. Ito (1996), Ising ; thickness $L_0 \leq 14$.

Improved Blume-Capel, $L_0 = 4$
$L = 8, 12, 16, 24, 32, 48, 64, 128$, and 256.



Fitting the data with the Ansatz

$$\bar{\beta}_{c,2D}(L_0, L) = \beta_{c,2D}(L_0) + cL^{-3}$$

we get, taking all data into account, $\beta_{c,2D}(4) = 0.43968710(12)$, $c = -0.080(1)$ and $\chi^2/\mathrm{d.o.f.} = 1.16$.

Similar results for $L_0 = 8$

We took results obtained for $L \gtrapprox 16L_0$ as our final estimate.

about 2 years of CPU time on a single core of a Quad-Core AMD Opteron(tm) 2378 CPU running at 2.4 GHz

L_0	L	$\beta_{c,2D}$	$-\frac{1}{L} \left.\frac{\partial R_Z}{\partial \beta}\right\|_{R_Z=R_Z^*}$
4	256	0.43968704(18)	2.5259(11)
5	160	0.4258884(15)	2.903(7)
6	384	0.41724094(59)	3.256(9)
7	112	0.4114039(17)	3.579(8)
8	512	0.40724571(12)	3.875(4)
9	300	0.40416349(61)	4.157(11)
10	256	0.40180434(69)	4.430(12)
11	256	0.39995347(66)	4.669(13)
12	192	0.39846789(82)	4.918(13)
13	192	0.39725856(81)	5.147(14)
14	256	0.39625624(59)	5.391(15)
15	256	0.39541461(57)	5.568(16)
16	256	0.39470035(55)	5.789(16)
17	256	0.39408852(54)	6.048(17)
24	384	0.39148514(31)	7.350(23)
25	384	0.39125639(31)	7.524(24)
32	512	0.39013763(21)	8.661(29)
48	768	0.38900912(12)	10.988(46)
64	1024	0.38854284(8)	12.973(52)
∞		0.387721735(25)	

Ansatz with an effective thickness $L_{0,eff} = L_0 + L_s$
(going back to Capehart and Fisher 1976)

$$\beta_{c,2D}(L_0) - \beta_{c,3D} = a[L_0 + L_s]^{-1/\nu}$$

fixing $\beta_{c,3D} = 0.387721735(25)$ and $\nu = 0.63002(10)$
Taking into account $L_0 \geq 24$ we still get $\chi^2/\text{d.o.f.} = 2.91$

$\Longrightarrow$ Add an t^2 correction:

$$\beta_{c,2D}(L_0) - \beta_{c,3D} = a[L_0 + L_s]^{-1/\nu} + b[L_0 + L_s]^{-2/\nu}$$

$L_{0,min}$	a	b	L_s	χ^2/d.o.f.
6	0.61841(5)	0.546(5)	0.9665(18)	3.41
7	0.61815(7)	0.505(9)	0.9570(29)	1.23
8	0.61813(7)	0.502(9)	0.9560(29)	1.12
9	0.61806(7)	0.485(12)	0.9513(37)	0.97
10	0.61799(8)	0.467(17)	0.9467(46)	0.85
11	0.61797(10)	0.462(22)	0.9453(61)	0.93
12	0.61791(11)	0.440(30)	0.9401(77)	0.91

From the magnetization profile of films with $(O, +)$ boundary conditions $L_s = 0.96(2)$

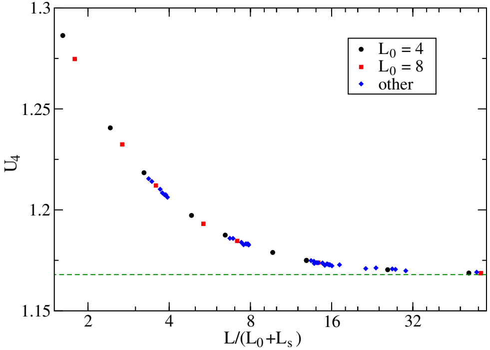
In terms of the scaling variable $x = t[L_0/\xi_0]^{1/\nu}$ where ξ_0 is the amplitude of the bulk correlation length in the high temperature phase and $t = \beta - \beta_{c,3D}$:

$$x_c = -a\xi_0^{-1/\nu} = -6.444(10)$$

Similar

$$\lim_{L_0 \to \infty} \frac{L_0}{\xi_{2nd,bulk}(\beta_{c,2D}(L_0))} = 6.27(2)$$

Check of 2D Ising Universality: U_4 at $\bar{\beta}(L_0, L)$



- Convergence consistent with $\omega_{eff} = 7/4$
- Similar behaviour can be observed for ξ_{2nd}/L

The standard Ising model. Blue numbers: H. Kitatani, M. Ohta, and N. Ito (1996)

L_0	L	β_c
2	64	0.3117590(11)
3	96	0.27524559(62)
4	256	0.25837693(38)
4		0.25844(4)
5	100	0.2488632(11)
6	120	0.24285524(82)
6		0.24289(3)
7	140	0.23877132(73)
8	256	0.23584204(16)
8		0.23587(2)
10	160	0.23197795(88)
10		0.23209(3)
12	192	0.22958611(36)
12		0.22965(3)
14		0.22804(3)
16	256	0.22685595(31)
20	320	0.22538715(25)
24	384	0.22449313(16)
28	448	0.22390290(26)
32	512	0.22348981(26)
36	576	0.22318793(23)
40	640	0.22295923(19)
48	768	0.22264034(17)
∞		0.22165462(2)

Fitting with

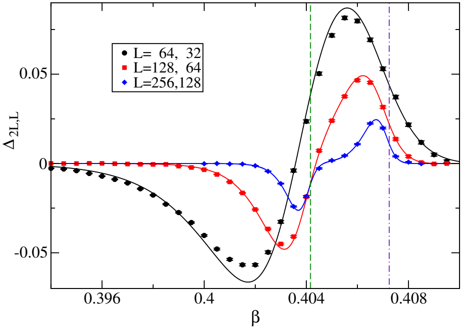
$$\beta_{c,2D}(L_0) - \beta_{c,3D} = a[L_0 + cL_0^{1-\omega} + L_s]^{-1/\nu} + b[L_0 + cL_0^{1-\omega} + L_s]^{-2/\nu}$$

we get $a = 0.4845(15)$. Using $\xi_0 = 0.1962(1)$ we arrive at

$$x_c = -a\xi_0^{-1/\nu_{3D}} = -6.426(25)$$

which is fully consistent with the Blume-Capel result.

Thermodynamic Casimir effect:



$\Delta_{2L,L} = \Delta E(L_0, 2L) - \Delta E(L_0, L)$ for $L_0 = 8.5$

For the matiching of the reduced temperatures we use the slope of R_Z at the critical point

Conclusions:

- Transition is in the universality class of the 2D Ising model
- $\beta_{c,2D}(L_0)$ approaches $\beta_{c,3D}$ as predicted by finite size scaling. For the lattice sizes studied here, corrections to scaling have to be taken into account.

M. Caselle and M. Hasenbusch, *Deconfinement Transition and Dimensional Crossover in the 3-D Gauge Ising Model*, [hep-lat/9511015], Nucl. Phys. B **470**, 435 (1996).

Martin Hasenbusch, *Thermodynamic Casimir Effect in Films: the Exchange Cluster Algorithm* arXiv:1410.7161

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