The thermodynamic Casimir effect: Monte Carlo simulations of improved three-dimensional lattice models

Martin Hasenbusch

Institut für Physik, Humboldt-Universität zu Berlin

Leipzig 24 November 2011

Overview

- Introduction
- Improved lattice models
- Numerical results
- Comparison with other MC studies and field theory

Work published as M.H. Phys. Rev. B 84, 134405 (2011)

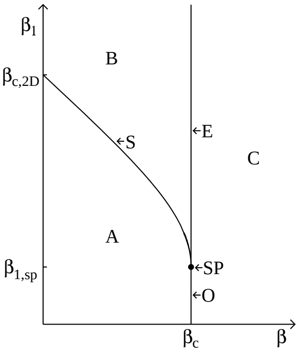
Reviews on surface critical phenomena:

K. Binder, in *Phase Transitions and Critical Phenomena, Vol. 8*,
H. W. Diehl, in *Phase Transitions and Critical Phenomena, Vol. 10*,
edited by C. Domb and J.L. Lebowitz

Three-dimensional semi-infinite Ising model, reduced Hamiltonian

$$H = -\beta \sum_{<xy>} s_x s_y - h \sum_x s_x - \beta_1 \sum_{<xy>\in S} s_x s_y - h_1 \sum_{x\in S} s_x \quad ,$$

Phase diagram for $h = h_1 = 0$



- A: Bulk and surface are disordered
- B: Bulk is disordered, surface is ordered
- C: Bulk and surface are ordered
- From A to C: Ordinary transition
- From B to C: Extraordinary transition
- From A to B: Surface transition
- SP: Special point (is a tricritical point)
- $h_1 \neq 0 \rightarrow$ extraordinary transition

Surface critical exponents govern the behaviour of surface quantities in the neighbourhood of the critical point:

$$m_1 \simeq t^{\beta_1} \qquad \chi_1 = \frac{\partial m_1}{\partial h} \simeq t^{-\gamma_1} \qquad \chi_{1,1} = \frac{\partial m_1}{\partial h_1} \simeq t^{-\gamma_{1,1}}$$

where m_1 is the magnetisation at the surface; Surface specific heat

$$C_s \simeq t^{-\alpha_s}$$

These exponents can be expressed in terms of the RG-exponents

At the ordinary transition: In addition to the relevant bulk RG-exponents y_t, y_h the surface RG-exponent y_{h_1} is relevant.

At the special point in addition y_{t_1}.

We study the Blume-Capel model on the simple cubic lattice:

$H = -\beta \sum_{<x,y>} s_x s_y + D \sum_x s_x^2$ where $s_x \in \{-1, 0, 1\}$

In the limit $D \to -\infty$ we get the Ising model; For $D < D_{tri}$ with $D_{tri} \approx 2.03$ line of second order phase transitions in the 3D Ising universality class.

Improved model:
At $D = 0.656(20)$ the amplitudes of corrections $\propto L^{-\omega}$ or $\propto t^{-\theta}$ vanish;

From finite size scaling study:
$\nu = 0.63002(10)$, $\eta = 0.03627(10)$ and $\omega = 0.832(6)$

$$\beta_c(D = 0.655) = 0.387721735(10)$$

See M.H., Phys. Rev. B 82, 174433 (2010)

Reduced Hamiltonian of the Blume-Capel model with film geometry

$$
\begin{aligned}
H &= -\beta \sum_{<xy>} s_x s_y + D \sum_x s_x^2 - h \sum_x s_x \\
&- \beta_1 \sum_{<xy>, x_0=y_0=1} s_x s_y - \beta_2 \sum_{<xy>, x_0=y_0=L_0} s_x s_y \\
&+ D_1 \sum_{x, x_0=1} s_x^2 + D_2 \sum_{x, x_0=L_0} s_x^2 \\
&- h_1 \sum_{x, x_0=1} s_x - h_2 \sum_{x, x_0=L_0} s_x
\end{aligned}
$$

$x = (x_0, x_1, x_2)$ with $1 \leq x_i \leq L_i$.

Periodic boundary conditions in 1 and 2-direction.

In our finite size scaling study $L = L_0 = L_1 = L_2$.

We study three different models

- Blume-Capel $D = 0.655$; $D_1 = D_2 = 0$
- Blume-Capel $D = 0.655$; $D_1 = D_2 = -\infty$
  (spins at the surfaces are fixed to $s = \pm 1$)
- Ising model

Simulation algorithm: Hybrid of cluster algorithm and local heatbath

We simulate at $\beta = \beta_c$, $h = h_1 = h_2 = 0$ and $\beta_1 = \beta_2 \approx \beta_{1,s}$,
lattice sizes up to $L = 128$
We compute the Taylor-series of observables in β_1 up to $O(\beta_1^3)$
around the simulation point.

For $L = 128$ we performed 2×10^8, 1.4×10^8, and 1.2×10^8
measurements, for the three models respectively

In total 12 years on one core of a 2.4 GHz CPU

Finite size scaling of RG-invariant quantities R:

- Ratio of partition functions Z_a/Z_p
- Binder cumulamt $U_4 =< m^4 > / < m^2 >^2$

$$R(\beta = \beta_c, \beta_1, h = 0, h_1 = 0) = g(c t_1 L^{y_{t_1}})$$

Determine $\beta_{1,s}$ with the standard crossing method

$$\bar{S} := \left. \frac{\partial R_1(\beta = \beta_c, \beta_1, h = 0, h_1 = 0)}{\partial \beta_1} \right|_{\beta_1 = \beta_{1,f}} \propto L^{y_{t_1}}$$

where $R_2(\beta = \beta_c, \beta_1 = \beta_{1,f}, h = 0, h_1 = 0) = R_{2,f}$
(See also talk of Francesco Parisen Toldin)

Ansaetze:

$$\bar{S} = cL^{y_{t_1}}$$

$$\bar{S} = cL^{y_{t_1}}(1 + dL^{-1})$$

$$\bar{S} = cL^{y_{t_1}}(1 + dL^{-1} + eL^{-2})$$

Corrections:

- $\propto L^{-1}$ due to the surfaces
- $\propto L^{-\omega'}$, $\omega' = 1.67(11)$, Newman and Riedel (1984)
- $\propto L^{-\omega''}$, $\omega'' \approx 2$, breaking of the rotational invariance by the lattice; analytic background in the magn. susceptibility
- and infinitely many more ...

Table: *Fitting the slope of Z_a/Z_p at $Z_a/Z_p = 0.3138$ for BC model with $D_1 = D_2 = 0$*

Ansatz	L_{min}	y_{t_1}	d	e	χ^2/DOF
1	32	0.71909(21)			4.26/3
1	48	0.71855(36)			0.89/2
2	12	0.71583(28)	–0.148(6)		20.91/5
2	16	0.71700(38)	–0.108(11)		1.57/4
3	8	0.71795(49)	–0.026(21)	–0.71(9)	5.39/5
3	12	0.71872(82)	0.022(49)	–1.01(30)	3.75/4

BC model with $D_1 = D_2 = -\infty$ gives consistent results
Results from Ising model deviate only slightly $\rightarrow$ residual leading corrections have little effect in case of the Blume Capel model.
Conclusion:

$$y_{t_1} = 0.718(2)$$

Behaviour of the surface susceptibility at the special point

$$\bar{\chi} := \chi|_{R=R_f} \propto L^{2y_{h_1}-2}$$

Ansaetze

$$\bar{\chi} = cL^x$$

$$\bar{\chi} = cL^x(1 + dL^{-1})$$

$$\bar{\chi} = cL^x(1 + dL^{-1}) + b$$

$$\bar{\chi} = cL^x(1 + dL^{-1} + eL^{-2}) + b$$

Table: *Fitting the surface susceptibilities χ_{11} and χ_{12} at $Z_a/Z_p = 0.3138$. Both the data for $D_1 = D_2 = 0$ and $D_1 = D_2 = -\infty$ are taken into account.*

Obs.	Ansatz	L_{min}	x	d_1	d_2	χ^2/DOF
$\bar{\chi}_{11}$	2	24	1.2930(3)	–0.09(1)	1.13(1)	10.37/7
$\bar{\chi}_{11}$	2	32	1.2932(4)	–0.09(2)	1.15(2)	4.48/5
$\bar{\chi}_{11}$	3	16	1.2935(4)	–0.08(5)	1.39(6)	6.87/7
$\bar{\chi}_{11}$	4	8	1.2933(6)	–0.19(15)	1.12(15)	8.56/9
$\bar{\chi}_{12}$	2	24	1.2921(2)	–0.36(1)	0.02(1)	4.01/7
$\bar{\chi}_{12}$	2	32	1.2922(3)	–0.35(1)	0.03(1)	2.96/5
$\bar{\chi}_{12}$	3	16	1.2932(4)	–0.19(6)	0.35(6)	10.28/7
$\bar{\chi}_{12}$	3	24	1.2927(5)	–0.25(12)	0.16(13)	3.10/5
$\bar{\chi}_{12}$	4	8	1.2935(2)	–0.13(2)	0.32(5)	14.61/9
$\bar{\chi}_{12}$	4	12	1.2929(3)	–0.30(4)	0.02(9)	7.83/7
$\bar{\chi}_{12}$	4	16	1.2928(6)	–0.14(17)	–0.06(25)	3.19/5

Conclusion: $x = 1.2929(10) \quad \rightarrow \quad y_{h_1} = 1.6465(6)$

At the ordinary transition: $y_{h_1} = 0.7249(6)$
M.H., Phys. Rev. B 83, 134425 (2011)

Comparison with previous results for the special point obtained by Monte Carlo simulations and field theoretic methods:

Ref.	year	Method	y_{h_1}	y_{t_1}
Binder, Landau	1984	MC	1.72(4)	0.89(6)
Binder, Landau	1990	MC	1.71(3)	0.94(6)
Vendruscolo et al.	1992	MC	1.65	1.17
Ruge et al.	1992	MC	1.624(8)	0.732(24)
Ruge, Wagner	1995	MC	1.623(2)	
Selke, Pleimling	1998	MC	1.635(16)	
Deng,Blöte,Nightingale	2005	MC	1.636(1)	0.715(1)
this work	2011	MC	1.6465(6)	0.718(2)
Reeve, Diehl, Dietrich	1981	ϵ-exp, naive	1.65	1.08
Diehl, Shpot	1998	ϵ-exp, res.		0.752
Diehl, Shpot	1994	3D-exp, res.	1.583	0.856

Conclusions:

The study of improved models allows to accurately determine critical exponents in the case of surface critical phenomena

In the presence of surfaces there are corrections $\propto L^{-1}$ corrections. These are difficult to disentangle from those $\propto L^{-\omega}$ which are present in the generic case.

In order to estimate systematic errors due to the (necessary) truncation of the Wegner series it is helpful to

- simulate several models
- study several observables
- use more than one Ansatz

This work was supported by the DFG under the Grant HA 3150/2-2

Thank you for your attention!