

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

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Overview

- ▶ Introduction
- ▶ Finite size scaling of the thermodynamic Casimir force
- ▶ Improved lattice models
- ▶ Numerical results
- ▶ Comparison with other MC studies, field theory and experiment

Hendrik Casimir 1948:

A force is caused by the **spatial restriction** of **quantum fluctuations**
In particular: There is an attractive force between two conducting parallel plates in the vacuum

M. E. Fisher and P.-G. de Gennes 1978:

Analogously to the Casimir effect, also the **spatial restriction** of **thermal fluctuations** causes a force. This effect is called the **thermodynamic** (or thermal, or critical) **Casimir effect**.

Experiments:

- ▶ Films of ^4He near the λ -transition
- ▶ Films of a $^3\text{He} - ^4\text{He}$ mixture near the tricritical point
- ▶ Films of binary mixtures near the mixing transition
- ▶ spheres immersed in binary mixture.

^4He and ^3He - ^4He mixture:

- ▶ R. Garcia and M. H. W. Chan,
Critical Fluctuation-Induced Thinning of ^4He Films near the Superfluid Transition, Phys. Rev. Lett. **83** (1999) 1187
- ▶ A. Ganshin, S. Scheidemantel, R. Garcia , and M. H. W. Chan,
Critical Casimir Force in ^4He Films: Confirmation of Finite-Size Scaling, Phys. Rev. Lett. **97** (2006) 075301
- ▶ R. Garcia and M. H. W. Chan,
Critical Casimir Effect near the ^3He - ^4He Tricritical Point, Phys. Rev. Lett. **88** (2002) 086101

binary liquid mixtures:

- ▶ M. Fukuto, Y. F. Yano and P. S. Pershan,
[Critical Casimir Effect in Three-Dimensional Ising Systems: Measurements on Binary Wetting Films](#)
Phys. Rev. Lett. **94** (2005) 135702
- ▶ C. Hertlein, L. Helden, A. Gambassi, S. Dietrich, and C. Bechinger, [Direct measurement of critical Casimir forces](#),
Nature 451, (2008) 172
- ▶ F. Soyka, O. Zvyagolskaya, C. Hertlein, L. Helden, C. Bechinger
[Critical Casimir Forces in Colloidal Suspensions on Chemically Patterned Surfaces](#) Phys. Rev. Lett. **101** (2008) 208301
- ▶ A. Gambassi, A. Maciołek, C. Hertlein, U. Nellen, L. Helden, C. Bechinger, and S. Dietrich,
[Critical Casimir effect in classical binary liquid mixtures](#)
Phys. Rev. **E** 80 (2009) 061143

Here throughout: **Film geometry**

System is **finite** in **one direction** (0-direction in the following) and **infinite** in the **other two** (1- and 2-direction)

The range of **thermal fluctuations** is characterized by the **correlation length** ξ . For $L_0 \lesssim \xi$ **fluctuations are restricted** by the film
 \implies a **force** $F_{Casimir}$ **per area** acts on the walls. It is given by

$$F_{Casimir} = -\frac{\partial \tilde{f}_{ex}(L_0)}{\partial L_0}$$

The **excess free energy** per area

$$\tilde{f}_{ex}(L_0) = \tilde{f}(L_0) - L_0 \tilde{f}_{bulk}$$

Finite size scaling predicts:

$$F_{Casimir} \simeq \frac{k_B T}{L_0^3} \theta(t[L_0/\xi_0]^{1/\nu})$$

where the function $\theta(x)$ is universal. Note that the correlation length behaves as $\xi \simeq \xi_0 t^{-\nu}$ and $t = (T - T_c)/T$ is the reduced temperature.

The universal function $\theta(x)$ depends on

- ▶ Universality class of the bulk system; Here: 3D Ising or 3D XY
- ▶ Surface universality classes of the two boundaries

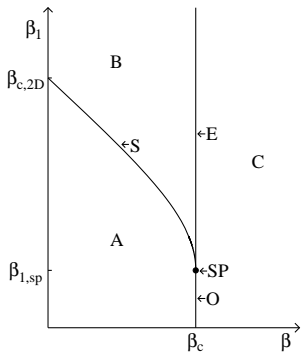
Corrections to finite size scaling $\propto L_0^{-\omega}$, $\propto L_0^{-2\omega}$, $\propto L_0^{-\omega'}$, ...,
where $\omega = 0.832(6)$ and $\omega' \approx 2\omega$

Corrections due to the surfaces $\propto L_0^{-1}$, ...

Three-dimensional semi-infinite Ising model, reduced Hamiltonian

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

Phase diagram for $h = h_1 = 0$

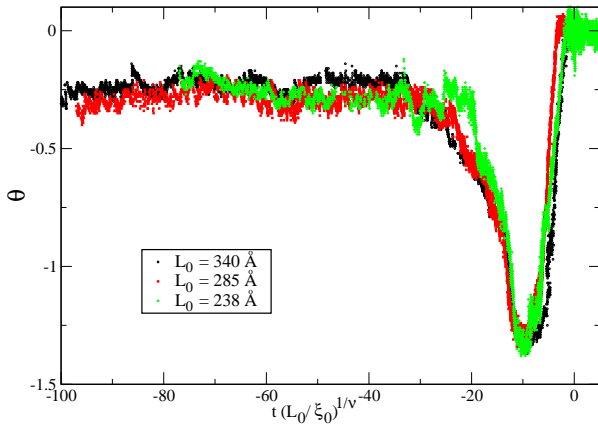


- ▶ A: Bulk and surface are disordered
- ▶ B: Bulk is disordered, surface is ordered
- ▶ C: Bulk and surface are ordered
- ▶ From A to C: Ordinary transition
- ▶ From B to C: Extraordinary transition
- ▶ From A to B: Surface transition
- ▶ SP: Special point
- ▶ $h_1 \neq 0 \rightarrow$ extraordinary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

Theoretical results for $\theta(x)$:

- ▶ Mean-field
- ▶ Exact results for the two-dimensional Ising model
- ▶ Field theoretic results for systems with periodic and anti-periodic boundary conditions and near the ordinary transition in the high temperature phase; More recently also near the special point
- ▶ de Gennes-Fisher local-functional method:
3D Ising systems with symmetry-breaking boundary conditions
- ▶ Monte-Carlo simulations

Chan et al (2006)
Films of ^4He



λ -transition of ^4He in the 3D XY universality class

No excess ordering at the boundaries \rightarrow ordinary transition

Lattice models:

- ▶ N -component ϕ^4 model:

$$H = -\beta \sum_{\langle x,y \rangle} \vec{\phi}_x \vec{\phi}_y + \sum_x \left[\vec{\phi}_x^2 + \lambda (\vec{\phi}_x^2 - 1)^2 \right]$$

where the field variable $\vec{\phi}_x$ is a vector with N real components.
 x, y are sites on a simple cubic lattice, $\langle xy \rangle$ is a pair of nearest neighbours.

The partition function is $Z = \left[\prod_x \prod_{i=1}^N \int d\phi_x^{(i)} \right] \exp(-H)$

$\lambda = 0$: Gaussian model; $\lambda \rightarrow \infty$: Ising, XY, Heisenberg, ..., model.

- ▶ Blume-Capel model: $H = -\beta \sum_{\langle x,y \rangle} s_x s_y + D \sum_x s_x^2$
where $s_x \in \{-1, 0, 1\}$

In the neighbourhood of a **second order phase transition**, e.g. the **correlation length** in the **thermodynamic limit** behaves as

$$\xi = \xi_{0,\pm}(\lambda) |t|^{-\nu} (1 + c_{\xi}(\lambda)t^{\nu\omega} + \dots)$$

Finite size scaling of the **Binder cumulant** $U_4 = \langle m^4 \rangle / \langle m^2 \rangle^2$ (similar ξ_{2nd}/L , Z_a/Z_p):

$$U_4|_{t=0} = U_4^* + c_U(\lambda)L^{-\omega} + \dots$$

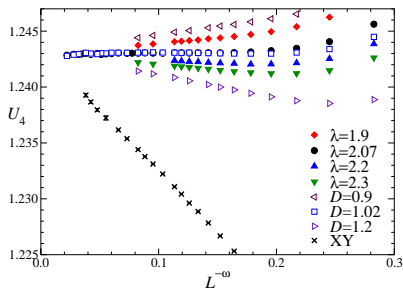
The **improved model**: $c_{\xi}(\lambda^*) = \dots = c_U(\lambda^*) = \dots = 0$

Idea: J.H. Chen, M. E. Fisher, and B. G. Nickel, Phys. Rev. Lett. 48, 630 (1982); M. E. Fisher and J. H. Chen, J. Physique (Paris) 46, 1645 (1985). See also K. Symanzik, Nucl. Phys. B 226, 187 (1983), Nucl. Phys. B 226, 205 (1983)

Numerical results $N = 2$:

M.H. and T. Török, J.Phys.A 32, 6361 (1999), M. Campostrini, M.H., A. Pelissetto, P. Rossi, E. Vicari, Phys.Rev.B 63, 214503 (2001), M. Campostrini, M.H., A. Pelissetto, E. Vicari, Phys. Rev. B 74, 144506 (2006).

U_4 at $Z_a/Z_p = 0.3202$



$\lambda^* = 2.15(5)$

Here we study $\lambda = 2.1$:

$\beta_c = 0.5091503(6)$,

$\xi_{0,+} = 0.26362(8)$,

$\left| \frac{c(2.1)}{c(XY)} \right| \lesssim \frac{1}{30}$

Numerical results $N = 1$:

H.G. Ballesteros, L.A. Fernandez, V. Martin-Mayor, G. Parisi, and

J.J. Ruiz-Lorenzo, J. Phys. A 32 (1999) 1: $\lambda^* \approx 1$

M. H., J.Phys.A 32, 4851 (1999): $\lambda^* \approx 1.1$

Blume-Capel model:

H.W.J. Blöte, E. Luijten and J.R. Heringa, J.Phys.A 28, 6289 (1995):

$D^* \approx \ln 2 = 0.6931\dots$

M.H., K. Pinn, S. Vinti, Phys.Rev.B 59, 11471 (1999): $D^* \approx 0.641$

M.H., Phys. Rev. B 82, 174433 (2010): $D^* = 0.656(20)$

We simulate at $D = 0.655$: $\beta_c = 0.387721735(25)$

Our results for critical exponents:

$\nu = 0.63002(10)$, $\eta = 0.03627(10)$ and $\omega = 0.832(6)$

For comparison: R. Guida, J. Zinn-Justin, J.Phys.A 31, 8103 (1998)

ϵ -expansion:

$\nu = 0.6305(25)$, $\eta = 0.0365(50)$ and $\omega = 0.814(18)$

Expansion for 3D fixed:

$\nu = 0.6304(13)$, $\eta = 0.0335(25)$ and $\omega = 0.799(11)$

How to compute $\partial f_{\text{ex}}/\partial L_0$?

Here we follow A. Hucht, Phys.Rev.Lett. 99, 185301 (2007):

On the lattice, we replace the partial derivative by a finite difference

$$\frac{\partial f_{\text{ex}}}{\partial L_0} \approx \Delta f_{\text{ex}} = f_{\text{ex}}(L_0 + 1/2) - f_{\text{ex}}(L_0 - 1/2)$$

For fixed λ or D :

$$\Delta f_{\text{ex}}(\beta) = - \int_{\beta_0}^{\beta} d\tilde{\beta} \Delta E_{\text{ex}}(\tilde{\beta})$$

where

$$\Delta E_{\text{ex}}(L_0) = E(L_0 + 1/2) - E(L_0 - 1/2) - E_{\text{bulk}}$$

with

$$E(L_0) = \frac{1}{L^2} \sum_{\langle x,y \rangle} \langle \vec{\phi}_x \vec{\phi}_y \rangle$$

How to chose β_0 ?

$\Delta E_{\text{ex}}(\beta)$ decays exponentially as $L_0/\xi \rightarrow \infty$. Therefore we chose β_0 such that $L_0 \gg \xi(\beta_0)$.

Numerical integration is done by using the **trapezoidal** rule:

$$\Delta f_{\text{ex}}(\beta_j) \approx - \sum_{i=1}^j \frac{1}{2} (\Delta E_{\text{ex}}(\beta_{i-1}) + \Delta E_{\text{ex}}(\beta_i)) (\beta_i - \beta_{i-1})$$

Number of **sampling points** ≈ 100 .

Numerical results:

- ▶ 3D XY universality class, free boundary conditions, $\beta_1 = 0$
(ordinary transition)
Comparison with experiments on ^4He films, field theoretic results
- ▶ 3D XY universality class, periodic boundary conditions
Comparison with field theoretic results
- ▶ 3D Ising universality class, symmetry breaking boundary conditions $(+, +)$ and $(+, -)$ (extraordinary transition)
Comparison with experiments on binary liquid mixtures, de Gennes Fisher local functional method
- ▶ 3D Ising universality class, crossover from ordinary to extraordinary

Monte Carlo simulation of the ϕ^4 model, $N = 2$, free or periodic boundary conditions:

Hybrid of the single cluster and Metropolis algorithm

- Bulk energy:

We simulate L^3 lattices with periodic boundary conditions

High temperature phase: finite size corrections decay exponentially with increasing L/ξ ; We simulate lattices with $L > 10\xi$.

Low temperature phase: Goldstone mode \rightarrow finite size corrections decay power-like; simulate lattices with different L and extrapolate

Neighbourhood of the critical point:

$$E(\beta) = E_{ns} + C_{ns}(\beta - \beta_c) + a_{\pm}|\beta - \beta_c|^{1-\alpha} + d_{ns}(\beta - \beta_c)^2 + b_{\pm}|\beta - \beta_c|^{2-\alpha}$$

Films undergo a **Kosterlitz-Thouless** phase transition in the **low temperature phase** of the bulk system at

$$x_{KT} = t_{KT}(L_0)[L_0/\xi_0]^{1/\nu} = -7.48(3) \quad (\text{free boundary conditions})$$

$$x_{KT} = t_{KT}(L_0)[L_0/\xi_0]^{1/\nu} = -2.86(2) \quad (\text{periodic boundary conditions})$$

in the limit $L_0 \rightarrow \infty$.

The correlation length of the film behaves as

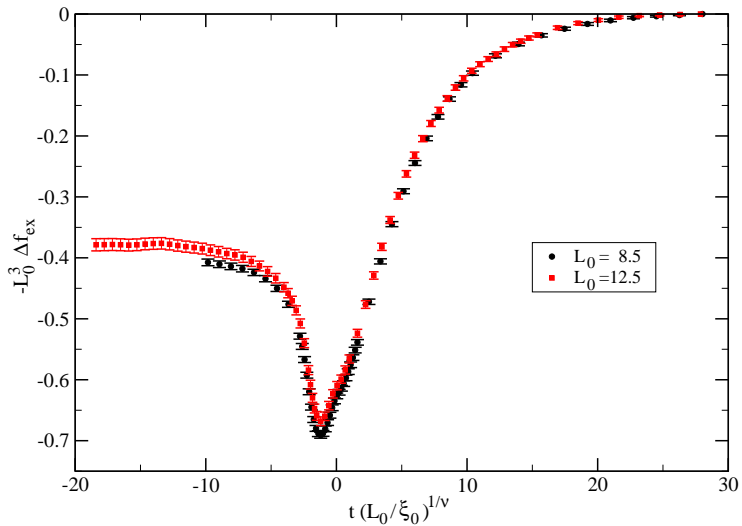
$$\xi_{film} \simeq c \exp(b[(x - x_{KT})/x_{KT}]^{-1/2})$$

The singular part of the free energy per area

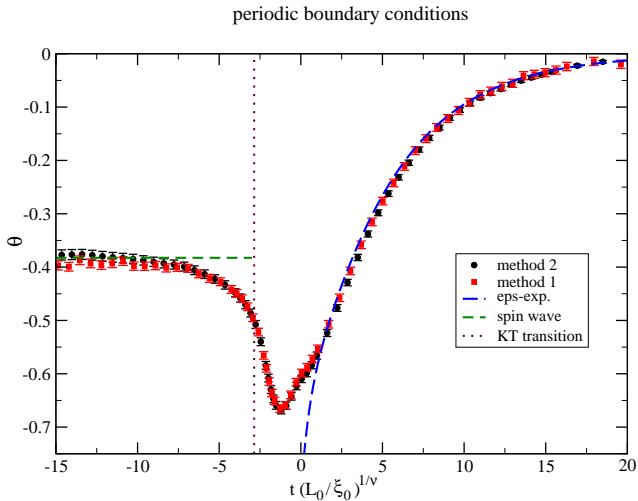
$$f_s \propto \xi_{film}^{-2} \simeq d \exp(-2b[(x - x_{KT})/x_{KT}]^{-1/2})$$

For $x < x_{KT}$ massless phase: **power-like** finite L corrections \rightarrow
Large L/L_0 are needed; We have simulated up to $L/L_0 = 128$

periodic boundary conditions



ϵ -expansion: Krech, Dietrich (1992), Grüneberg, Diehl (2008)



Comparison with Monte Carlo simulations of the XY model:

Our result for the **minimum** of $\theta(x)$:

$$x_{min} = -1.20(5) \text{ and } \theta_{min} = -0.66(2)$$

At the bulk critical point:

$$\theta(0) = -0.60(2)$$

Vasilyev, Gambassi, Maciolek and Dietrich (2008):

Qualitative agreement of the curve with our curve

$$x_{min} = -0.73(1) \text{ and } \theta_{min} = -0.633(1)$$

$$\theta(0) = -0.5986(14)$$

Free boundary conditions:

Renormalization group arguments: corrections $\propto L_0^{-1}$ can be written be expressed by an effective thickness:

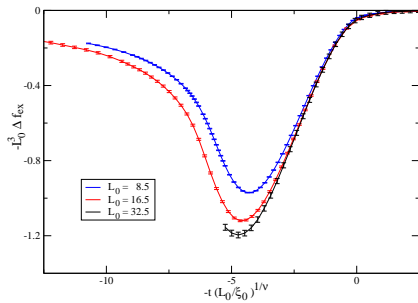
$$L_0 \rightarrow L_{0,eff} + L_s$$

We determine L_s from finite size scaling at the critical point, e.g.

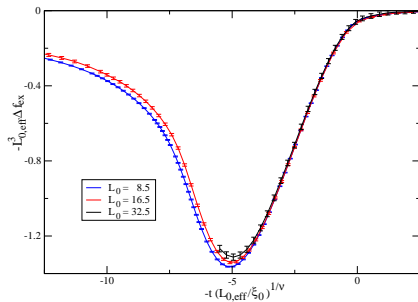
$$\xi_{film} = c(L_0 + L_s)$$

with c and L_s as free parameters. We get

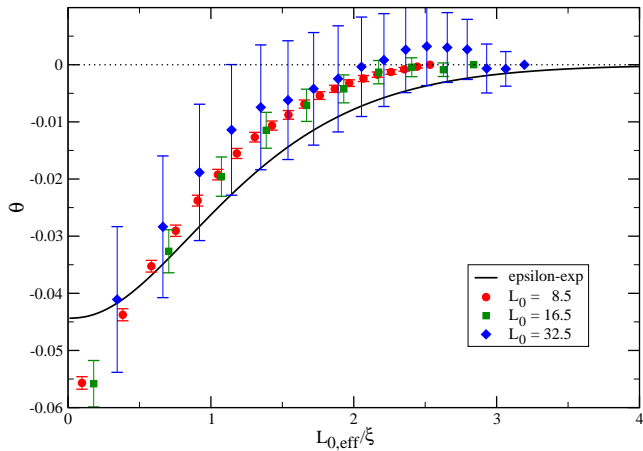
$$L_s = 1.02(7)$$



Our numerical results



ϵ -expansion: Krech and Dietrich (1992)



Comparison with Monte Carlo simulations of the XY model:

Our result for the **minimum** of θ :

$$x_{min} = -4.95(3) \text{ and } \theta_{min} = -1.31(1)$$

Hucht (2007)

Qualitative agreement of the curve with ours

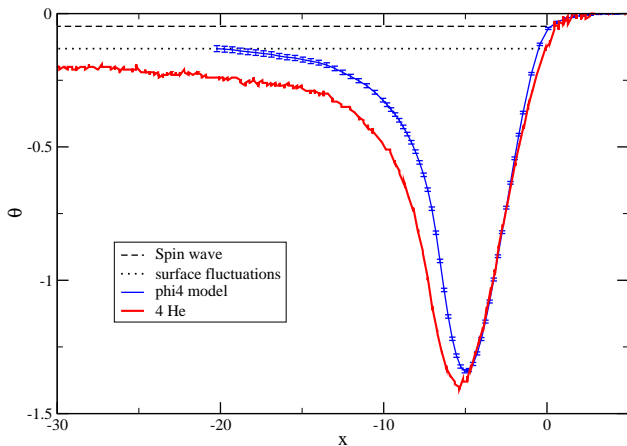
$$x_{min} = -5.3(1) \text{ and } \theta_{min} = -1.35(3)$$

Vasilyev, Gambassi, Maciolek and Dietrich (2008)

Qualitative agreement of the curve with ours

$$x_{min} = -5.43(2) \text{ and } \theta_{min} = -1.260(5)$$

Comparison with experiment:
Ganshin, Scheidemantel, Garcia, and Chan (2006)



Liquid binary mixture:

Typically a surface is more attractive to one of the two fluids than to the other → **symmetry breaking** boundary conditions (equivalent to the **extraordinary transition**)

Here we fix the spins at the surfaces to **+1** or **-1**.

Two principle alternatives: **(+, +)** or **(+, -)** boundary conditions.

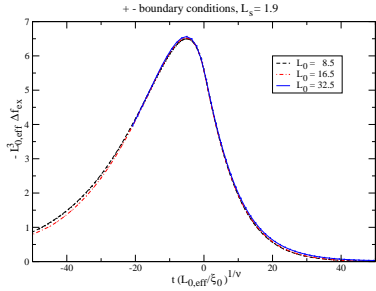
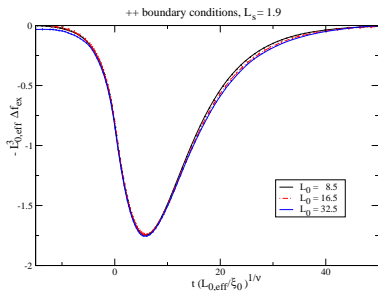
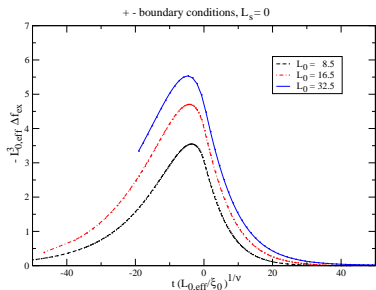
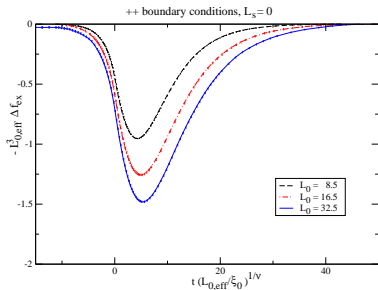
Simulation:

Cluster algorithm; local Heatbath/Metropolis; Multispin coding

Note: **no phase transition** for a finite thickness of the film.

For **(+, +)**, $\xi_{film}/L_0 < 0.15$ remains quite small for any temperature;

(+, -) low temperature phase: effectively described by a squeezed interface model; ξ_{film} increases as we go deeper into the low temperature phase



Comparison with other studies:

(+,+)

Our result: $x_{min} = 5.82(10)$, $\theta_{min} = -1.76(3)$

Dietrich et al (2009): $x_{min} = 5.98(8)$, $\theta_{min} \approx -1.4, -1.65, -1.8$,
depending on the ansatz for corrections to scaling

(+,-)

Our result: $x_{max} = -5.17(7)$, $\theta_{max} = 6.56(10)$, $\theta(0) = 5.613(20)$

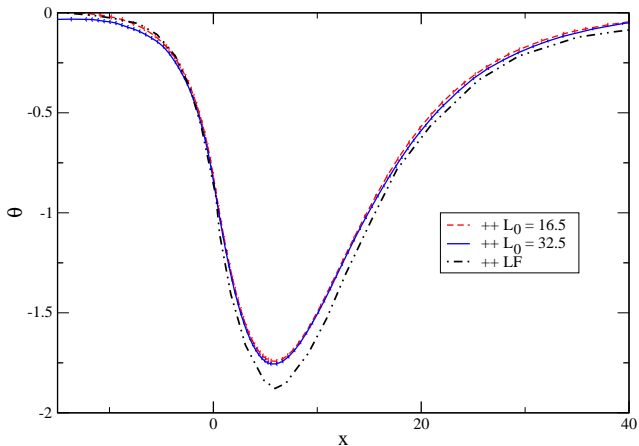
Dietrich et al (2009): $x_{max} = -5.4(1)$, $\theta_{max} \approx 5.3, 6.2, 7.1$,
depending on the ansatz for corrections to scaling
 $\theta(0) = 5.42(4)$, other ansaetze give $\theta(0) \approx 4.5, 6$.

Experiment: $\theta(0) = 6(2)$

de Gennes-Fisher local functional method

$$f = \int_0^{L_0} dx_0 \left[\frac{a}{2} \frac{d^2 m(x_0)}{dx_0^2} + V(m(x_0)) \right]$$

LF: Z. Borjan, P.J. Upton, Phys.Rev.Lett.101, 125702 (2008)

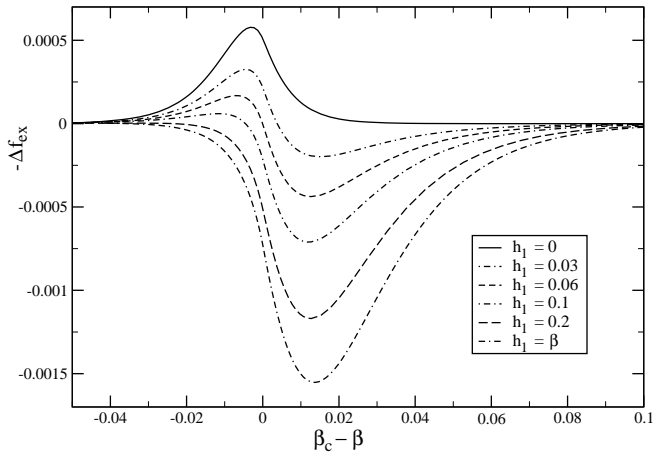


Crossover:

- ▶ ordinary to extraordinary
- ▶ special to ordinary
- ▶ special to extraordinary

Interesting feature: The thermodynamic Casimir force might **change sign** as a function of temperature or thickness of the film

We have studied film with spins fixed to **+1** at one surface and a weak symmetry breaking field **h_1** at the other.



Conclusion:

The **finite size scaling** function θ for experimentally relevant boundary condition can be **computed accurately** by the Monte Carlo simulation of improved models

Outlook:

Film: Consider boundary conditions corresponding to the special point and crossover special point to ordinary and extraordinary

Other geometries: Plate-Sphere; Sphere-Sphere

Thanks: DFG, Grants HA 3150/2-1, HA 3150/2-2