Thermodynamic Casimir Forces between a Sphere and a Plate: Monte Carlo Simulation of a Spin Model

Martin Hasenbusch

Institut für Physik, Humboldt-Universität zu Berlin

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Overview

- Introduction
- Improved Blume-Capel model
- Exchange cluster algorithm
- Numerical results
- Comparison with the Derjaguin approximation

Work published as M.H., [arXiv:1210.3961]

Introduction

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

spatial restriction of thermal fluctuations leads to an effective force (analogous to the Casimir force). Thermal fluctuations are long ranged near a critical point

Therefore thermodynamic, thermal or critical Casimir effect

Experiments:
Plate-plate (or film) geometry

- films of ^{4}He and mixtures of ^{3}He and ^{4}He near the λ-transition
- fluid binary mixture near the mixing-demixing transition

Plate-sphere geometry
Colloidal particle submersed in a fluid binary mixture

The thermodynamic Casimir force follows (finite size) scaling laws:

Film geometry

$$F_C \simeq k_B T L^{-d}\, \theta(t[L/\xi_{0,+}]^{1/\nu})$$

F_C: Casimir force per area, L: thickness of the film, correlation length in the high temperature phase $\xi \simeq \xi_{0,+} t^{-\nu}$, where $t = (T - T_c)/T_c$ is the reduced temperature, $\theta(x)$ is a universal function that depends on the universality classes of the bulk and the two surfaces.

Sphere-plate geometry

$$F_C(D, R, T) = \frac{k_B T}{R} K(t[D/\xi_{0,+}]^{1/\nu}, \Delta)$$

F_C: Casimir force, R: radius of the sphere, D: distance between sphere and plate, $\Delta = D/R$ and $K(x, \Delta)$ is a universal function

Universal functions $\theta(x)$ and $K(x, \Delta)$ can be computed by:

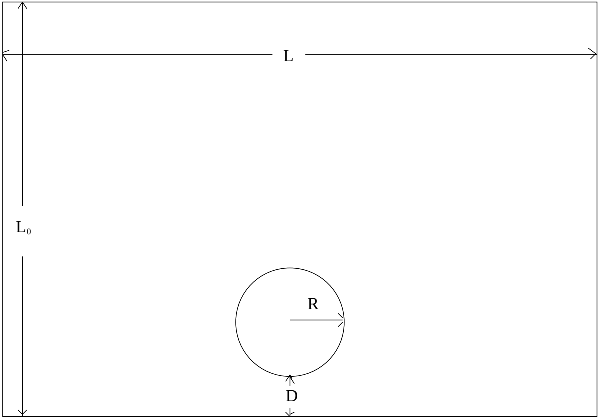
- Meanfield theory
- Exact results for 2 D Ising

Film geometry:

- field theoretic methods (rather restricted)
- Monte Carlo simulations of spin models by various groups in the last few years; Results for most experimentally interesting cases.

Plate-sphere geometry:

- small sphere expansion for $\Delta \gg 1$
- Derjaguin approximation for $\Delta \ll 1$ using $\theta(x)$ as input
- Monte Carlo simulations: Topic of the present talk



Idea case: infinitely large half-space above the plane

In the simulation finite extension $L_0, L \gg R, D$

We study strongly symmetry breaking boundary conditions

In the spin model $s_x = 1$ or $s_x = -1$ at the boundaries

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

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

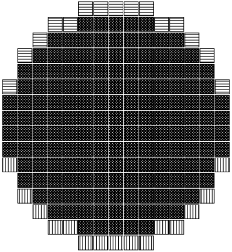
In the limit $\tilde{D} \to -\infty$ we get the Ising model; For $\tilde{D} < \tilde{D}_{tri}$ with $\tilde{D}_{tri} \approx 2.03$ line of second order phase transitions in the 3D Ising universality class.

Improved model:
At $\tilde{D} = 0.656(20)$ 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 $\omega = 0.832(6)$

$$\beta_c(\tilde{D} = 0.655) = 0.387721735(10)$$

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



Lattice approximation of a sphere (disc). Here two spheres, relative shift: one lattice spacing
Dark squares: Intersection of the two discs

The thermodynamic Casimir force is given by

$$\beta F_C(D,R,\beta) = -\frac{\partial F(D,R,\beta)}{\partial D}$$

$F(D,R,\beta)$ reduced free Energy. On the lattice:

$$\frac{\partial F(D,R,\beta)}{\partial D} \approx \Delta F(D,R,\beta) = F(D+1/2,R,\beta) - F(D-1/2,R,\beta)$$

Similar to Hucht, PRL **99**, 185301 (2007) we compute

$$\Delta F(D, R, \beta) = -\int_{\beta_0}^{\beta} \mathrm{d}\tilde{\beta} \Delta E(D, R, \tilde{\beta})$$

where

$$\Delta E(D, R, \beta) = E(D + 1/2, R, \beta) - E(D - 1/2, R, \beta)$$

and

$$E(D, R, \beta) = \sum_{<xy>} \langle s_x s_y \rangle_{D,R,\beta}$$

we chose β_0 such that $\Delta E(D, R, \beta) \approx 0$ which is given for $\xi \ll D$

Problem: $\langle s_x s_y \rangle_{D+1/2,R,\beta} - \langle s_x s_y \rangle_{D-1/2,R,\beta} \approx 0$ for x, y far away from the sphere.

However these distances contribute to the variance of $\Delta E(D, R, \beta)$.

Therefore for $L_0, L \gg R, D$ it is difficult to obtain $\Delta E(D, R, \beta)$ accurately from Monte Carlo simulations.

Way out: Exchange cluster algorithm (geometric cluster algorithm)
Heringa and Blöte, PRE **57**, 4976 (1998)

Simulate two systems with distances $D - 1/2$ and $D + 1/2$ simultaneously.
"Flipping a cluster": For all sites x in the cluster

$$s'_{x,1} = s_{x,2} \qquad s'_{x,2} = s_{x,1}$$

Can be done as single cluster (Wolff), Swendsen-Wang ...

In the construction of clusters a link $< xy >$ is "deleted" with the probability (taken from Heringa and Blöte)

$$p_d = \min\left[1, \exp\left(-\beta[s_{x,1} - s_{x,2}][s_{y,1} - s_{y,2}]\right)\right]$$

and "frozen" otherwise.

As usual, two sites belong to the same cluster if they are connected by a chain of frozen links.

We flip all clusters that do not contain "frozen sites"

x is a frozen site if $s_{x,1}$ or $s_{x,2}$ is fixed.

$$\Delta E(D,R,\beta) \approx$$

$$\frac{1}{2N}\sum_{i=1}^{N}[E^{(i+1)}(D+1/2,R,\beta) - E^{(i)}(D-1/2,R,\beta)$$

$$+E^{(i)}(D+1/2,R,\beta) - E^{(i+1)}(D-1/2,R,\beta)]$$

The exchange cluster leads to cancellations

$$E^{(i+1)}(D+1/2,R,\beta) - E^{(i)}(D-1/2,R,\beta)$$

$$= \sum_{<xy>, x \,\mathrm{or}\, y \in C_f} [s^{(i+1)}_{x,D+1/2} s^{(i+1)}_{y,D+1/2} - s^{(i)}_{x,D-1/2} s^{(i)}_{y,D-1/2}]$$

where C_f is a frozen cluster

We simulate systems with
$D = D_{min} - 1/2, D_{min} + 1/2, ..., D_{max} - 1/2, D_{max} + 1/2$
simulataneously to compute the thermodynamic Casimir force at
$D = D_{min}, D_{min} + 1, ..., D_{max} - 1, D_{max}$

Similar to parallel tempering, where one swaps the temperature and not the configuration, we actually exchange the frozen clusters and the distance of the sphere and not the complement of the frozen clusters.

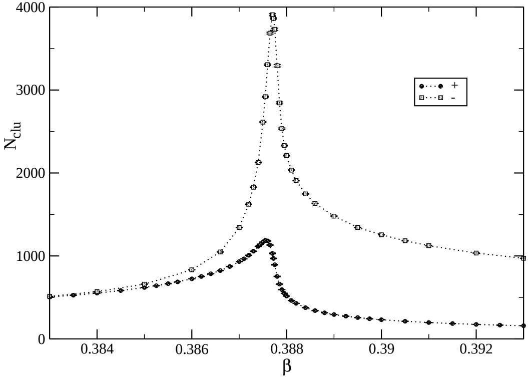
To get an ergodic algorithm we perform

- Swendsen-Wang cluster updates
- Heatbath updates

in addition to the exchange cluster update.

Furthermore:
frequent heatbath updates of a sub-lattice around the spheres

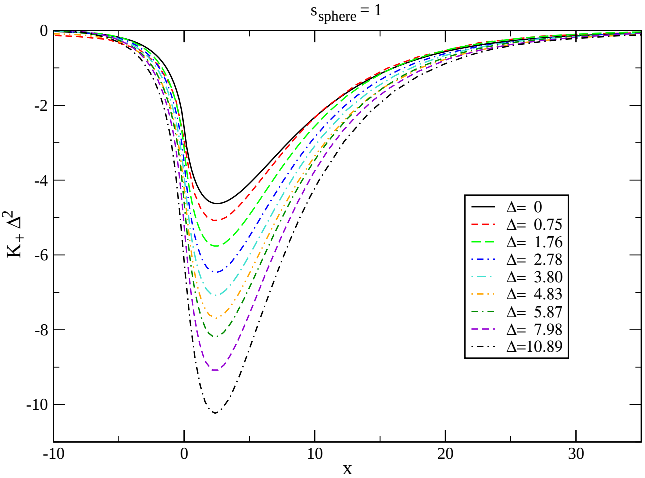
- $R = 7.5$, $D = 32$, Volume $298 \times 160^2 = 7628800$
- Boundary conditions $s_x = 1$ for $x_0 = 0$ and $x_0 = L_0 + 1$
- Spins of the sphere $s_x = s_{sphere}$ with $s_{sphere} = \pm 1$

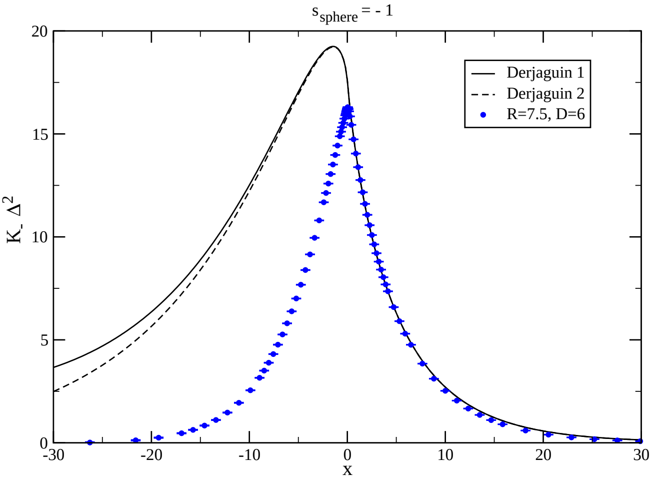


Size N_{clu} of the frozen clusters stays small compared with the volume;
However dependence on the parameters not well understood yet.

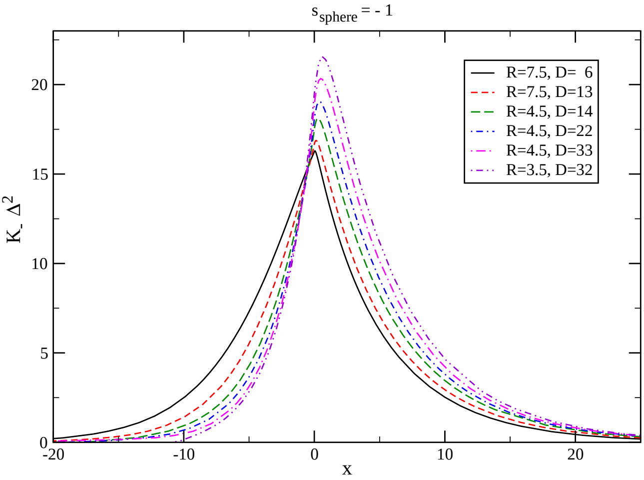
$K(0,\Delta) \propto \Delta^{-2}$ for $\Delta \ll 1$

$K(0,\Delta) \propto \Delta^{-1-\beta/\nu}$ for $\Delta \gg 1$ where $\beta/\nu \approx 0.5181$





$s_{sphere} = -1$
Derjaguin 1
Derjaguin 2
R=7.5, D=6
$K_- \Delta^2$
x
20
15
10
5
0
-30
-20
-10
0
10
20
30



$s_{sphere} = -1$
R=7.5, D= 6
R=7.5, D=13
R=4.5, D=14
R=4.5, D=22
R=4.5, D=33
R=3.5, D=32
K_ Δ^2
0
5
10
15
20
-20
-10
0
10
20
x

Conclusions and outlook:

- The exchange cluster algorithm allows to accurately compute the thermodynamic Casimir force between a sphere and a plane for a lattice spin model.
- We have computed the scaling functions $K_{\pm}(x, \Delta)$ for $1 \lessapprox \Delta \lessapprox 12$
- To optimise the algorithm we need better understanding of its behaviour
- Study other types of boundary conditions
- Study plate-plate and sphere-sphere geometry

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Thank you for your attention!