The thermodynamic Casimir effect in the neighbourhood of the  $\lambda$ -transition: A Monte Carlo study

#### Martin Hasenbusch

Institut für Physik, Humboldt-Universität zu Berlin

CompPhys10, Leipzig, 25 November 2010

The thermodynamic Casimir effect in the neighbourhood of the  $\lambda$ -transition: A Monte Carlo study

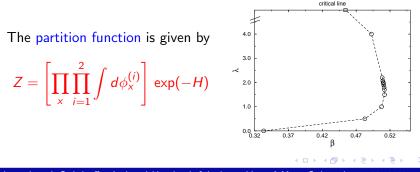
# Overview

- An improved lattice model
- Finite size scaling of the thermodynamic Casimir force
- Numerical results
- Comparison with other MC studies, field theory and experiment

2-component  $\phi^4$  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  $\mu$  direction.  $\lambda = 0$ : Gaussian model;  $\lambda \to \infty$ : XY model.



The thermodynamic Casimir effect in the neighbourhood of the  $\lambda$ -transition: A Monte Carlo study

The correlation length behaves as

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

where  $t = \beta_c - \beta$  is the reduced temperature.  $\theta = \nu \omega \approx 0.5$  is the exponent of leading corrections.

The improved model:  $c(\lambda^*) = 0$  Numerically:  $\lambda^* = 2.15(5)$ 

Here we study  $\lambda = 2.1$ :

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

The thermodynamic Casimir effect in the neighbourhood of the  $\lambda$ -transition: A Monte Carlo study

イロト イロト イヨト イヨト

## Film geometry:

System is finite in one direction and infinite in the other two In our simulations:  $L_0 \ll L_1 = L_2$ 

The range of fluctuations is characterized by the correlation length  $\xi$ . For  $L_0 \leq \xi$  fluctuations are restricted by the geometry of the film

 $\implies$  a force  $F_{Casimir}$  per area acts on the walls of the film.

《曰》《聞》《臣》《臣》 三臣

## Boundary conditions:

- periodic boundary conditions: theoretically relatively simple; no experimental realization
- free boundary conditions: Dirichlet boundary conditions with vanishing order parameter; relevant for films of <sup>4</sup>He in the neighbourhood of the λ-transition.

Corrections  $\propto L_0^{-1}$ ; Can be cast into the form  $L_{0,eff} = L_0 + L_s$ . For our model  $L_s = 1.02(7)$ . (Obtained from the numerical study of other quantities) The thermal (or critical) Casimir force is given by

$$F_{Casimir} = -\frac{\partial f_{ex}}{\partial L_0}$$

where  $L_0$  is the thickness of the film. The excess free energy per area:

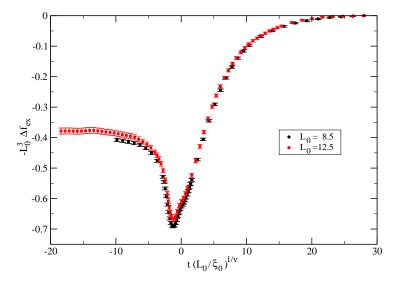
 $f_{ex} = f(L_0) - L_0 f_{bulk}$ 

Finite size scaling predicts:

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

where the function  $\theta(x)$  is universal

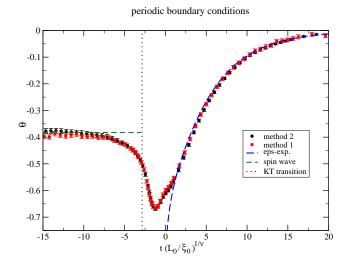
periodic boundary conditions



Martin Hasenbusch

< 67 >

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



The thermodynamic Casimir effect in the neighbourhood of the  $\lambda$ -transition: A Monte Carlo study

Comparison with Monte Carlo simulations of the XY model:

Our result for the minimum of  $\theta(x)$ :  $x_{min} = -1.20(5)$  and  $\theta_{min} = -0.66(2)$ 

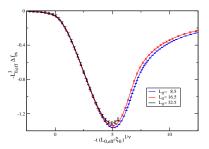
At the bulk critical point:  $\theta(0) = -0.60(2)$ 

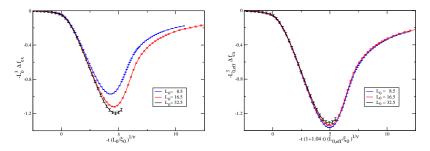
Vasilyev, Gambassi, Maciolek and Dietrich (2008): Qualitative agreement of the curve with our curve  $x_{min} = -0.73(1)$  and  $\theta_{min} = -0.633(1)$ 

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

(1日) (日) (日) (日)

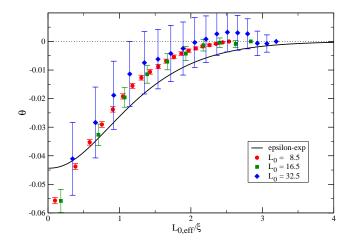
# Free boundary conditions





The thermodynamic Casimir effect in the neighbourhood of the  $\lambda$ -transition: A Monte Carlo study

# $\epsilon$ -expansion: Krech and Dietrich (1992)



The thermodynamic Casimir effect in the neighbourhood of the  $\lambda$ -transition: A Monte Carlo study

Martin Hasenbusch

< 67 ►

Comparison with Monte Carlo simulations of the XY model:

Our result for the minimum of  $\theta$ :  $x_{min} = -4.95(3)$  and  $\theta_{min} = -1.31(1)$ 

Hucht (2007) Qualitative agreement of the curve with ours  $x_{min} = -5.3(1)$  and  $\theta_{min} = -1.35(3)$ 

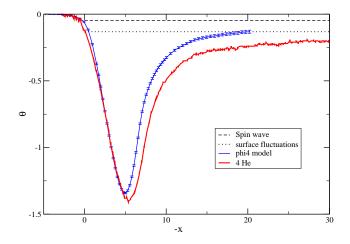
Vasilyev, Gambassi, Maciolek and Dietrich (2008) Qualitative agreement of the curve with ours  $x_{min} = -5.43(2)$  and  $\theta_{min} = -1.260(5)$ 

The thermodynamic Casimir effect in the neighbourhood of the  $\lambda$ -transition: A Monte Carlo study

Martin Hasenbusch

マボン イヨン イヨン 二日

Comparison with experiment: Garcia, Chan (1999), Ganshin, Scheidemantel, Garcia, and Chan (2006)



- M. H., The specific heat, the energy density and the thermodynamic Casimir force in the neighbourhood of the lambda-transition, [arXiv:0907.2847], accepted for publication in Phys.Rev.B
- M. H., Another method to compute the thermodynamic Casimir force in lattice models [arXiv:0908.3582] Phys.Rev.E 80 (2009) 061120
- M. H., The thermodynamic Casimir effect in the neighbourhood of the lambda-transition: A Monte Carlo study of an improved three dimensional lattice model, [arXiv:0905.2096], J. Stat. Mech. (2009) P07031
- M. H., The specific heat of thin films near the lambda-transition: A Monte Carlo study of an improved three-dimensional lattice model, [arXiv:0904.1535] J. Stat. Mech. (2009) P10006

- (目) - (日) - (日)