The specific heat, the energy density and the thermodynamic Casimir force in the neighbourhood of the \( \lambda \)-transition

Martin Hasenbusch

Institut für Physik, Humboldt-Universität zu Berlin
Newtonstr. 15, 12489 Berlin, Germany
e–mail: Martin.Hasenbusch@physik.hu-berlin.de

Abstract

We discuss the relation of the specific heat, the energy density and the thermodynamic Casimir effect in the case of thin films in the three dimensional XY universality class. The finite size scaling function \( \theta(x) \) of the thermodynamic Casimir force can be expressed in terms of the scaling functions \( h'(x) \) and \( h(x) \) of the excess energy density and the excess free energy density. A priori these quantities depend on the reduced temperature \( t \) and the thickness \( L_0 \) of the film. However finite size scaling theory predicts that the scaling functions depend only on the combination \( x = t[L_0/\xi_0]^{1/\nu} \), where \( \nu \) is the critical exponent and \( \xi_0 \) the amplitude of the correlation length. We exploit this fact to compute \( \theta \) from Monte Carlo data for the excess energy density of the improved two-component \( \phi^4 \) model on the simple cubic lattice with free boundary conditions in the short direction. We repeat this exercise using experimental data for the excess specific heat of \(^4\text{He} \) films. The finite size scaling behaviour of the excess specific heat is governed by \( h''(x) \), which is proportional to the scaling function \( f_2 \) discussed in the literature. We compare our results with previous work, where the Casimir force has been computed by taking the derivative of the excess free energy with respect to the thickness of the film. As a preparative study we have also computed the scaling functions \( h'(x) \) and \( h(x) \) for finite \( L^3 \) systems with periodic boundary conditions in all directions, where \( L \) is the linear extension of the system.

Keywords: \( \lambda \)-transition, Classical Monte Carlo simulation, thin films, finite size scaling, thermodynamic Casimir effect
1 Introduction

In 1978 Fisher and de Gennes \[1\] realized that when thermal fluctuations are restricted by a container a force acts on the walls of the container. Since this effect is rather similar to the Casimir effect, where the restriction of quantum fluctuations induces a force, it is called “thermodynamic” Casimir effect. Since thermal fluctuations only extend to large scales in the neighbourhood of a continuous phase transitions it is also called “critical” Casimir effect. Recently this effect has attracted much attention, since it could be verified for various experimental systems and quantitative predictions could be obtained from Monte Carlo simulations of spin models \[2\].

In the thermodynamic limit of the three dimensional system, the correlation length, which measures the spatial extension of fluctuations, diverges following the power law

\[
\xi \simeq \xi_0,\pm |t|^{-\nu}
\]

where \( t = (T - T_c)/T_c \) is the reduced temperature and \( T_c \) the critical temperature. \( \xi_0,\pm \) are the amplitudes of the correlation length in the high and low temperature phase, respectively. While \( \xi_0,\pm \) depend on the microscopic details of the system, the critical exponent \( \nu \) and the ratio \( \xi_0,+/\xi_0,- \) are universal.

At the critical point also other quantities like the specific heat show a singular behaviour:

\[
C \simeq A_{\pm} |t|^{-\alpha} + B.
\]

In the case of the XY universality class that we consider here, the exponent \( \alpha = -0.151(3) \) \[3\] of the specific heat is negative. Therefore the analytic background \( B \) has to be taken into account. Note that the critical exponents of the correlation length and the specific heat are related by the hyperscaling relation \( \alpha = 2 - d\nu \), where \( d \) is the dimension of the system. For reviews on critical phenomena and its modern theory, the Renormalization Group, see e.g. \[4, 5, 6, 7\].

The singular behaviour at the critical point originates from the fact that thermal fluctuations range over all length scales. Therefore the behaviour in the neighbourhood of the critical point is modified if the system is confined by a container. A priori thermodynamic quantities are functions of the reduced temperature and the size \( L_0 \) of the container, assuming a fixed geometry. However the theory of finite size scaling \[4\] predicts that the physics of the system is governed by the ratio \( L_0/\xi \) as long as \( L_0,\xi \gg a \), where \( a \) is the microscopic scale of the system. In particular if

\[1\] For a review on finite size scaling see \[8\].
a quantity in the thermodynamic limit behaves as \( A \simeq a_0, |t|^{-w} \), finite size scaling predicts that \( A(L_0, t) \simeq L_0^{w/\nu} g(L_0/\xi) \), where \( w \) is the critical exponent of \( A \) and \( \xi \) the correlation length of the bulk system. We can rewrite this equation as

\[
A(L_0, t) \simeq L_0^{w/\nu} g(t[L_0/\xi_0]^{1/\nu})
\]

by using (1), which is the form used in the following. Note that the function \( g \) depends on the details of the container. For example for a cube it is different from a thin film. It also depends on the type of boundary conditions that is imposed by the walls of the container on the order parameter of the system.

The predictions of finite size scaling theory have been tested in experiments and theoretical studies for various universality classes and confining geometries; for reviews see [8, 9]. Here we shall focus on thin films in the three dimensional XY universality class, which is shared by the \( \lambda \)-transition of \(^4\)He. Very precise experimental results for critical exponents and universal amplitude ratios were obtained for this phase transition [10]. Also a large number of experiments on thin films of \(^4\)He and \(^3\)He-\(^4\)He mixtures were performed to probe finite size scaling [11]. In particular the specific heat \( C \) of thin films has been studied. The excess specific heat should behave as

\[
C_{\text{bulk}}(t) - C(L_0, t) \simeq L_0^{w/\nu} f_2(t[L_0/\xi_0]^{1/\nu})
\]

The reason to study the excess specific heat rather than just the specific heat \( C(L_0, t) \) is to cancel the analytic background \( B \). Note that the scaling function \( f_2(x) \) of the excess specific heat is, up to a constant factor, the second derivative \( h''(x) \) of the scaling function \( h(x) \) of the excess free energy per area

\[
\tilde{f}_{\text{ex}} = \tilde{f}_{\text{film}}(L_0, t) - L_0 \tilde{f}_{\text{bulk}}(t) \simeq k_B T L_0^{-d+1} h(x)
\]

where \( \tilde{f}_{\text{film}}(L_0, t) \) is the free energy per area of the thin film, \( \tilde{f}_{\text{bulk}}(t) \) the free energy density of the bulk system, \( d = 3 \) the dimension of the system and \( x = t[L_0/\xi_0]^{1/\nu} \). Note that in the case of thin films we consider, following the literature on the thermodynamic Casimir effect, free energies per area. We hope that this does not lead to confusion, since in the case of the specific heat, energies per volume are considered.

From a thermodynamic point of view, the Casimir force per unit area is given by

\[
F_{\text{casimir}} = - \frac{\partial \tilde{f}_{\text{ex}}}{\partial L_0}
\]
where $L_0$ is the thickness of the film. Inserting the finite size scaling ansatz (5) for the excess free energy into (6) we get

\[
F_{\text{casimir}} \simeq -k_B T \frac{\partial \left[ L_0^{-2} h(t[L_0/\xi_0]^{1/\nu}) \right]}{\partial L_0}
\]

\[
= -k_B T L_0^{-3} \left[ -2h(t[L_0/\xi_0]^{1/\nu}) + \frac{1}{\nu} t[L_0/\xi_0]^{1/\nu} h'(t[L_0/\xi_0]^{1/\nu}) \right]
\]

\[
= k_B T L_0^{-3} \sigma(t[L_0/\xi_0]^{1/\nu})
\]

(7)

where

\[
\sigma(x) = 2h(x) - \frac{x}{\nu} h'(x).
\]

This relation is well known and can be found e.g. in [14]. We like to emphasis, that it is at the very heart of finite size scaling that the behaviour of the Casimir force, which gives the reaction of the film with respect to a change of the thickness and the excess specific heat which gives the reaction of the film with respect to a change of the temperature are given by the same scaling function $h(x)$ of the excess free energy.

The purpose of the present work is to compute the finite size scaling function $\theta(x)$ by using the energy density of thin films obtained from Monte Carlo simulations of a lattice model [15] and by using experimental data for the specific heat of thin films of $^4$He near the $\lambda$-transition [16, 17].

As a preliminary study, we simulate $L^3$ systems with periodic boundary conditions in all directions. In order to eliminate leading corrections to scaling we have used the improved two component $\phi^4$ model on the simple cubic lattice. For a precise definition of the model see section 2. Using the results obtained for the energy density for a dense grid of temperatures in the neighbourhood of the critical point, we investigate the scaling behaviour and compute the finite size scaling functions $h'(x)$ and $h(x)$. We find that corrections to scaling are small for the lattices sizes $L = 8, 16$ and $32$ that we have simulated.

In the case of thin films we analyse data for the energy density that were obtained in [15] from simulations of the improved two component $\phi^4$ model on the simple cubic lattice. In [15] these data where used to compute the specific heat. In order to get a vanishing order parameter as it is observed at the boundaries of $^4$He films, Dirichlet boundary conditions with vanishing field were imposed. In singular quantities these lead to corrections $\propto L_0^{-1}$ [18], which can be expressed by an effective thickness $L_{0,\text{eff}} = L_0 + L_s$. In [19] we find $L_s = 1.02(7)$ for the model that we consider here. Note that the boundary conditions also effect the
analytic background of the specific heat and the energy density, which also leads to corrections $\propto L_0^{-1}$. However it turns out that these corrections are not given by the same $L_{0,\text{eff}}$ as for the singular quantities. Taking into account these subtleties we arrive at accurate result for $h'(x)$, $h(x)$ and $\theta(x)$. In particular for $\theta(x)$ in the range $-15 \lesssim x \lesssim 4$ we find a good match with our previous result $[20]$ where we computed the Casimir force by taking the derivative of the excess free energy with respect to the thickness $L_0$ of the film.

Next we compute $\theta(x)$ by using experimental results for the excess specific heat obtained from experiments on thin films of $^4$He $[16, 17]$. Even though this is a quite simple exercise, to our knowledge, it has not been done before. For $-5 \lesssim x \lesssim 4$ we find a reasonable match with our result $[20]$. However in the low temperature phase, for $x \lesssim -5$ we get results that strongly deviate from $[20]$ and can be ruled out by plausibility. This corroborates the observation that in the low temperature phase for $x \lesssim -5$ the excess specific heat does not scale well $[11]$.

This paper is organized as follows: First we define the model and the observables that we consider. Next we discuss the finite size scaling behaviour of the free energy density. In particular, we discuss corrections to scaling caused by Dirichlet boundary conditions. In section 4 we compute the scaling functions $h'(x)$ and $h(x)$ for $L^3$ systems with periodic boundary conditions. Then in section 5 we compute $h'(x)$, $h(x)$ and $\theta(x)$ using the data for the energy density of thin films with Dirichlet boundary conditions obtained in $[15]$. The result for $\theta(x)$ is compared with the one that we $[20]$ obtained directly from the thermodynamic Casimir force. Next in section 6 we compute $\theta(x)$ starting from data for the excess specific heat of films of $^4$He in the neighbourhood of the $\lambda$-transition. Finally we summarize and conclude.

## 2 The model and the observables

We study the two component $\phi^4$ model on the simple cubic lattice. We label the sites of the lattice by $x = (x_0, x_1, x_2)$. The components of $x$ might assume the values $x_i \in \{1, 2, \ldots, L_i\}$. In this work we have performed simulations of lattices with $L_0 = L_1 = L_2$ and periodic boundary conditions in all three directions. Furthermore we analyse data obtained in $[15]$ for thin films. In this case lattices of the size $L_1 = L_2 = L$ and $L_0 \ll L$ are studied. In 1 and 2-direction periodic boundary conditions and free boundary conditions in 0-direction are employed. This means

\[\text{In $[20]$ we have compared our result for $\theta(x)$ with previous ones obtained from simulations of the XY model $[21, 22]$ and experiments on thin films of $^4$He $[12, 13]$; overall we find a reasonable agreement.}\]
that the sites with $x_0 = 1$ and $x_0 = L_0$ have only five nearest neighbours. This type of boundary conditions could be interpreted as Dirichlet boundary conditions with $0$ as value of the field at $x_0 = 0$ and $x_0 = L_0 + 1$. Note that viewed this way, the thickness of the film is $L_0 + 1$ rather than $L_0$. This provides a natural explanation of the result $L_s = 1.02(7)$ obtained in [19]. The Hamiltonian of the two component $\phi^4$ model, for a vanishing external field, is given by

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

(9)

where the field variable $\vec{\phi}_x$ is a vector with two real components. $<x,y>$ denotes a pair of nearest neighbour sites on the lattice. The partition function is given by

$$Z = \prod_x \left[ \int d\phi_x^{(1)} \int d\phi_x^{(2)} \right] \exp(-\mathcal{H}).$$

(10)

Note that following the conventions of our previous work, e.g. [23], we have absorbed the inverse temperature $\beta$ into the Hamiltonian. In the limit $\lambda \to \infty$ the field variables are fixed to unit length; i.e. the XY model is recovered. For $\lambda = 0$ we get the exactly solvable Gaussian model. For $0 < \lambda \leq \infty$ the model undergoes a second order phase transition that belongs to the XY universality class. Numerically, using Monte Carlo simulations and high-temperature series expansions, it has been shown that there is a value $\lambda^* > 0$, where leading corrections to scaling vanish. Numerical estimates of $\lambda^*$ given in the literature are $\lambda^* = 2.10(6)$ [21], $\lambda^* = 2.07(5)$ [23] and most recently $\lambda^* = 2.15(5)$ [3]. The inverse of the critical temperature $\beta_c$ has been determined accurately for several values of $\lambda$ using finite size scaling (FSS) [3]. We shall perform our simulations at $\lambda = 2.1$, since for this value of $\lambda$ comprehensive Monte Carlo studies of the three-dimensional system in the low and the high temperature phase have been performed [19, 3, 25, 26]. At $\lambda = 2.1$ one gets $\beta_c = 0.5091503(6)$ [3]. Since $\lambda = 2.1$ is not exactly equal to $\lambda^*$, there are still corrections $\propto L^{-\omega}$, although with a small amplitude. In fact, following [3], it should be by at least a factor 20 smaller than for the standard XY model.

In [19] we find for $\lambda = 2.1$ by fitting the data for the second moment correlation length in the high temperature phase $\xi_{2nd} \simeq 0.26362(8)t^{-0.6717}$, where $t = 0.5091503 - \beta$. We shall use this definition of the reduced temperature also in the following discussion of our numerical results; Hence $\xi_0 = 0.26362(8)$. Note that in the high temperature phase there is little difference between $\xi_{2nd}$ and the

\[^3\text{Therefore, following [6] we actually should call it reduced Hamiltonian.}\]
exponential correlation length \( \xi_{\text{exp}} \) which is defined by the asymptotic decay of the two-point correlation function. Following \[23\] \( \lim_{t \to 0} \xi_{\text{exp}}^{2} = 1.000204(3) \) for the thermodynamic limit of the three-dimensional system. Hence at the level of precision reached here it does not matter whether \( \xi_{0,\text{exp}} \) or \( \xi_{0,2nd} \) is used in the scaling variable \( x = t|L_{0}/\xi_{0}|^{1/\nu} \).

### 2.1 The internal energy and the free energy

The reduced free energy density is defined as

\[
f = -\frac{1}{L_{0}L_{1}L_{2}} \log Z .
\]

I.e. compared with the free energy density \( \tilde{f} \), a factor \( k_{B}T \) is skipped.

Note that in eq. (9) \( \beta \) does not multiply the second term. Therefore, strictly speaking, \( \beta \) is not the inverse of \( k_{B}T \). In order to study universal quantities it is not crucial how the transition line in the \( \beta-\lambda \) plane is crossed, as long as this path is not tangent to the transition line. Therefore, following computational convenience, we vary \( \beta \) at fixed \( \lambda \). Correspondingly we define the (internal) energy density as the derivative of the reduced free energy density with respect to \( \beta \). Furthermore, to be consistent with our previous work \[15\], we multiply by \(-1\):

\[
E = \frac{1}{L_{0}L_{1}L_{2}} \frac{\partial \log Z}{\partial \beta} .
\]

It follows

\[
E = \frac{1}{L_{0}L_{1}L_{2}} \left\langle \sum_{<x,y>} \vec{\phi}_{x} \cdot \vec{\phi}_{y} \right\rangle ,
\]

which can be easily determined in Monte Carlo simulations. From eqs. (11,12) it follows that the free energy density can be computed as

\[
f(\beta) = f(\beta_{0}) - \int_{\beta_{0}}^{\beta} d\tilde{\beta} E(\tilde{\beta}) .
\]

### 3 The finite size scaling behaviour of the free energy

Let us briefly discuss the scaling behaviour of the reduced excess free energy per area. Since we study an improved model we ignore corrections \( \propto L_{0}^{-\omega} \) in the following. We take into account leading corrections due to the boundary conditions by
replacing the thickness $L_0$ of the film by $L_{0,\text{eff}} = L_0 + L_s$ at the appropriate places. We split the free energies in singular (s) and non-singular (ns) parts:

$$f_{\text{ex}}(t, L_0) = f_{\text{film}}(t, L_0) - L_0 f_{\text{bulk}}(t)$$

$$= f_{\text{film},s}(t, L_0) + L_{0,\text{eff},\text{ns}} f_{\text{ns}}(t) - L_0 f_{\text{bulk},s}(t) - L_0 f_{\text{ns}}(t)$$

$$= L_{0,\text{eff}} h(x) + L_s(t) f_{\text{bulk},s}(t) + L_{\text{ns}}(t) f_{\text{ns}}(t)$$

(15)

where

$$h(x) = L_{0,\text{eff}}^2 [f_{\text{film},s}(t, L_0) - L_{0,\text{eff}} f_{\text{bulk},s}(t)]$$

(16)

is a universal finite size scaling function and $x = t[L_{0,\text{eff}}/\xi_0]^{1/\nu}$. Following RG theory the non-singular part is not affected by finite size effects. However it is not clear a priori how Dirichlet boundary conditions affect the non-singular part of the free energy. Therefore we allow for $L_{\text{ns}} = L_{0,\text{eff},\text{ns}} - L_0 \neq 0$ and $L_{\text{ns}} \neq L_s$. Taking the derivative with respect to $L_0$ we get the thermodynamic Casimir force per area

$$\beta F_{\text{casimir}} = \frac{\partial f_{\text{ex}}(t, L_0)}{\partial L_0} = 2L_{0,\text{eff}}^{-3} h(x) - L_{0,\text{eff}}^{-3} \frac{1}{\nu} x h'(x) = L_{0,\text{eff}}^{-3} \theta(x)$$

(17)

where

$$\theta(x) = 2h(x) - \frac{1}{\nu} x h'(x).$$

(18)

Note that the boundary terms $L_s f_{\text{bulk},s}$ and $L_{\text{ns}} f_{\text{ns}}$ do not contribute to the Casimir force.

4 Warmup exercise: finite cubic system with periodic boundary conditions

First we have studied a finite lattice with $L = L_0 = L_1 = L_2$ with periodic boundary conditions in all directions. This way we avoid corrections caused by the free boundary conditions and possible difficulties related with the Kosterlitz-Thouless transition of thin films. In our simulations we determine the energy density $E$ for the lattice sizes $L = 8, 16$ and $32$ for a large number of $\beta$-values in the neighbourhood of the critical temperature. In particular, we have simulated at 159 $\beta$-values in the interval $0.35 \leq \beta \leq 0.58$, 205 $\beta$-values in the interval $0.35 \leq \beta \leq 0.58$ and 161 $\beta$-values in the interval $0.45 \leq \beta \leq 0.535$ in the case of $L = 8, 16$ and $32$, respectively. For most of these simulations we performed $10^6$ measurements. For
each of these measurements we performed one Metropolis sweep, two overrelaxation sweeps and a number of single cluster \[27\] updates. The number of single cluster updates is chosen such that the number of updates times the average size of a cluster roughly equals \(L^3\). As random number generator we have used the SIMD-oriented Fast Mersenne Twister algorithm \[28\]. In total we have used about 3 weeks of CPU-time on a single core of a Quad-Core Opteron(tm) 2378 CPU (2.4 GHz). In order to compute the excess energy density

\[
E_{\text{ex}}(L, t) = E(L, t) - E_{\text{bulk}}(t)
\]  

we have used the results for \(E_{\text{bulk}}(t)\) obtained in section 4.1 of \[15\].

The reduced excess free energy density behaves as

\[
f(t, L) - f_{\text{bulk}}(t) \simeq L^{-3} h(x)
\]  

(20)

where \(x = t[L/\xi_0]^{1/\nu}\). It follows for the excess energy density

\[
E(t, L) - E_{\text{bulk}}(t) \simeq [L/\xi_0]^{1/\nu} L^{-3} h'(x)
\]  

(21)

Since we study an improved model and periodic boundary conditions in all directions, we expect that analytic corrections are leading. In figure \[1\] we plot \([L/\xi_0]^{-1/\nu} L^3 [E(t, L) - E_{\text{bulk}}(t)]\) as a function of \(t[L/\xi_0]^{-1/\nu}\). The curves for \(L = 8, 16\) and 32 fall nicely on top of each other, showing that corrections to scaling are numerically small. The excess energy is positive for all temperatures. At \(x \approx -0.3\) the function assumes a maximum. The value at the maximum is \(\approx 0.295\). In the high temperature phase, for increasing \(x\) the function \(h'(x)\) rapidly approaches zero. In contrast, in the low temperature phase it is only slowly approaching zero with decreasing \(x\). This behaviour might be explained by the presence of a Goldstone mode in the low temperature phase.

Next we have computed the excess free energy using eq. (14). To this end we integrated our data for the excess energy by using the trapezoidal rule. We have started the integration at \(\beta_0 = 0.35, 0.45\) and 0.49 for \(L = 8, 16\) and 32, respectively. At these values of \(\beta_0\) the deviation of the excess energy from zero is of similar size as the statistical error. In figure \[2\] we plot \(L^3 [f(t, L) - f_{\text{bulk}}(t)]\) as a function of \(t[L/\xi_0]^{-1/\nu}\). As one should expect, the curves for \(L = 8, 16\) and 32 fall nicely on top of each other. Since the excess energy is positive for all values of \(x\), the excess free energy is monotonically increasing with increasing \(x\). At the critical point the scaling functions assumes the value \(h(0) = -1.162(4)\).

In Fig. 6 of \[29\] results for an isotropic \(L^3\) system with periodic boundary conditions for the Ising universality class and the limit \(n \to \infty\) of \(O(n)\) symmetric
Figure 1: We consider an $L^3$ system with periodic boundary conditions in all directions. We plot $[E(t, L) - E_{\text{bulk}}(t)][L/\xi_0]^{-1/\nu}L^3$ as a function of $t(L/\xi_0)^{1/\nu}$ for $L = 8, 16$ and $32$, where we use $\nu = 0.6717$ and $\xi_0 = 0.26362$. For a discussion see the text.
Figure 2: We consider an $L^3$ system with periodic boundary conditions in all directions. We plot $L^3[f(t, L) - f_{bulk}(t)]$ as a function of $t(L_0/\xi_0)^{1/\nu}$ for $L_0 = 8, 16$ and 32, where we use $\nu = 0.6717$ and $\xi_0 = 0.26362$. For a discussion see the text.
models are given. The Ising result is obtained from a perturbative approach in three dimensions fixed, while the $n \to \infty$ result is exact. In the Ising case, $h(x)$ shows a minimum in the low temperature phase, while for $n \to \infty$ it is monotonically decreasing as the temperature decreases. Hence qualitatively the behaviour for $n = 2$, studied here, is the same as for $n \to \infty$.

5 Film geometry with free boundary conditions

Here we study thin films with free boundary conditions in the short direction. This geometry is relevant for the comparison with experimental results obtained for thin films of $^4\text{He}$. Most of the Monte Carlo data are taken from our previous work \[15, 20\], where we have simulated films of the thicknesses $L_0 = 8, 16$ and $32$. Therefore we refrain from giving the details of the simulations and refer the reader to \[15, 20\].

Analogous to the previous section we compute the scaling function $h'(x)$ of the excess energy density and $h(x)$ of the excess free energy density. Using these we obtain the scaling function $\theta(x) = 2h(x) - \frac{x}{\nu}h'(x)$ of the thermodynamic Casimir force.

In \[15\] we have taken great care to get the deviations of the energy density from its effectively two dimensional thermodynamic limit under control. In order to achieve this, quite large ratios $L_1/L_0$ are needed in the neighbourhood of the peak of the specific heat. In the case of $L_0 = 8$ we have simulated lattices of a size up to $L_1 = L_2 = 2048$, and for $L_0 = 16$ up to $L_1 = L_2 = 1800$. For $L_0 = 32$ we have skipped the interval $0.5136 < \beta < 0.516$, since we could not simulate sufficiently large values of $L_1 = L_2$.

In figure 3, similar to the previous section, we have plotted $E_{ex}L_0^2[L_0/\xi_0]^{-1/\nu}$ versus $t[L_0/\xi_0]^{1/\nu}$, where now

$$E_{ex}(L_0, t) = L_0[E(L_0, t) - E_{bulk}(t)]$$

is the excess energy per area. In contrast to the previous section we find that there is a huge discrepancy between the three curves. The dominant effect seems that the curves are shifted by a constant with respect to each other. Note that replacing $L_0$ by $L_{0,eff} = L_0 + L_s$ with $L_s = 1.02(7)$ \[19\] does change this situation only little. In section \[3\] we have argued that the analytic background of the energy density might suffer from a boundary correction that is not given by the effective thickness $L_{0,eff} = L_0 + L_s$ that describes the leading boundary corrections of singular quantities. Below we shall study this question in detail at the critical point of the bulk system, where we have data for thicknesses up to $L_0 = 64$ available.
Figure 3: We plot $E_{ex} L_0^2 [L_0/\xi_0]^{-1/\nu}$ as a function of $t[L_0/\xi_0]^{1/\nu}$ for thin films, where we have used $\xi_0 = 0.26362$ and $\nu = 0.6717$. For a discussion see the text.
Table 1: Energy density of thin films of the thickness $L_0$ at the inverse critical temperature $\beta_c = 0.5091503(6)$ of the three dimensional systems. In all cases $L_1 = L_2 = 6L_0$.

| $L_0$ | $E$           |
|------|---------------|
| 8    | 0.799566(31)  |
| 12   | 0.832786(19)  |
| 16   | 0.850727(13)  |
| 24   | 0.8698028(85) |
| 32   | 0.8798552(57) |
| 48   | 0.8903321(37) |
| 64   | 0.8957662(29) |

5.1 Finite Size Scaling at the critical point of the bulk system

In order to get a better understanding of the corrections we have studied in detail the behaviour at the critical point of the three dimensional bulk system. In the context of [15] we have simulated lattices of the thickness $L_0 = 8, 12, 16, 24, 32, 48$ and $64$ and $L_1 = L_2 = 6L_0$. In [15] we have checked that this choice of $L_1, L_2$ is sufficient to approximate well the effectively two dimensional thermodynamic limit of the film at the critical point of the three dimensional system. Our results for the energy density are summarized in table 1.

In the case of periodic boundary conditions in all directions, the energy density at the critical point behaves as

$$E(L) = E_{ns} + cL^{-d+1/\nu} \quad (23)$$

where $d = 3$ is the dimension of the system. Using lattices of the size $L_0 = L_1 = L_2$ with $L_0$ up to 128 we find [25]

$$E_{ns} = 0.913213(5) + 20 \times (\beta_c - 0.5091503) + 5 \times 10^{-7} \times (1/\alpha + 1/0.0151). \quad (24)$$

In order to take into account corrections due to the free boundary conditions of the thin film we use the ansatz

$$L_0E(L_0) = (L_0 + L_{sns})E_{ns} + c_f L_0^{-d+1+1/\nu} \quad (25)$$
to fit the data given in table 1. As input we have used \( \nu = 0.6717(1) \) [3], \( E_{ns} \) given in eq. (24) and \( L_s = 1.02(7) \) [19]. The parameters of the fit are \( L_{sns} \) and \( c_f \). Fitting all data with \( L_0 \geq 8 \) we get an acceptable \( \chi^2/d.o.f. \). We find \( L_{ns} = -1.3529(3) \) when fixing \( L_s = 1.02 \) and \( L_{ns} = -1.3523(3) \) fixing \( L_s = 0.95 \). Hence \( L_{sns} \) is clearly different from \( L_s \) and it shows little dependence on the value taken for \( L_s \). We have checked that the error of \( L_{sns} \) due to the uncertainties of \( \nu \) and \( E_{ns} \) can be ignored.

5.2 Taking into account boundary corrections

The boundary correction \( L_{ns}E_{ns} \) should be an analytic function of the reduced temperature. In a first attempt we shall approximate it by its value at the critical point of the three dimensional system found above. Hence in figure 4 we plot \( \tilde{\mathcal{E}}_e L^2_{0,\text{eff}} / \xi_0^{1-1/\nu} \) for \( \mathcal{E}_{ex}(t) = L_0 E(L_0, t) - L_0,\text{eff} E_{\text{bulk}}(t) + (L_s - L_{sns})E_{ns} \) as a function of \( x = t[L_0,\text{eff}/\xi_0]^{1/\nu} \). Now we see a quite good matching of the three curves. Only for small \( x \) discrepancies are visible.

Next we have computed the finite size scaling function \( \theta \) of the Casimir force following eq. (18). In the case of \( L_0 = 8 \) and \( L_0 = 16 \) we have used the function \( h'(x) \) as given in figure 4. In the case of \( L_0 = 32 \) we have taken the missing part in the range \(-5.9 > x > -9.1\) from the results for \( L_0 = 16 \). To this end we have matched the values of the function at \( x = -5.9 \) and \( x = -9.1 \) resulting in \( h'_{32}(x) = h'_{16}(x) + 0.011 - 0.002(x + 5.9) \) for \(-5.9 > x > -9.1\). We have computed the function \( h(x) \) by numerically integrating \( h'(x) \) using the trapezoidal rule. For sufficiently large \( x \) the Casimir force vanishes and therefore \( h(x) = \frac{c}{2^\nu} h'(x) \). Hence for large \( x \):

\[
h'(x) = cx^{2\nu-1}.
\]

In [20] we found that the thermodynamic Casimir force is of similar size or smaller than the numerical errors that we achieve for \( x \gtrsim 4 \). We have checked that in this range the scaling function \( h'(x) \) of the excess energy indeed follows eq. (27).

Hence we have started the numerical integration in the high temperature phase at \( x_0 \approx 4 \) with the starting value \( h(x_0) = \frac{c}{2^\nu} h'(x_0) \). In order to check the reliability of our result, we have redone the integration using a set of data points, where we have skipped every second value of \( \beta \). We found an agreement within the statistical errors. Our results for \( \theta \) are plotted in figure 5. In the range \(-7 < x < 5 \) the curves obtained from the different values of \( L_0 \) match quite well. There is also a good match with \( \theta \) obtained in [20]. In particular the value and the position of
Figure 4: We plot $\tilde{E}_{ex} L_{0,\text{eff}}^2 [L_{0,\text{eff}}/\xi_0]^{-1/\nu}$ as a function of $t [L_{0,\text{eff}}/\xi_0]^{1/\nu}$ for $L_0 = 8$, 16 and 32. For a discussion see the text.
the minimum of $\theta$ are completely consistent. However for $x < -7$ the difference between the curves becomes clearly visible and increases with decreasing $x$. For small $x$, even for $L_0 = 32$ there is a huge discrepancy with the result of [20].

Since these discrepancies appear for large values of $|x|$ it is likely that they are mainly caused by analytic corrections. To check this explicitly, we allowed for two different types of corrections:

$$x = t(1 - ct)[L_{0,eff}/\xi_0]^{1/\nu}$$

and for a temperature dependence of the boundary correction of the analytic part of the energy

$$\bar{E}_{ex} = L_0E(L_0, t) - L_{0,eff}E_{bulk}(t) + (L_s - L_{sns})E_{ns} - c_0t.$$  

We find that the curves for $h'(x)$ obtained from $L_0 = 16$ and $L_0 = 32$ can be nicely matched by adjusting the two parameters $c$ and $c_b$. Matching in the interval $-18 < x < 3$ we find $c \approx -1.1$ and $c_b \approx -3.03$ and for the interval $-25 < x < 5$ $c \approx -0.75$ and $c_b \approx -2.97$. Using the corresponding results for $h'(x)$ we have computed the finite size scaling function $\theta(x)$ that is plotted in figure 6. Now we see that the rage of the matching with our previous result [20] is extended to $-15 \geq x \geq 4$ in the case of the matching range $-25 < x < 4$. For still smaller values of $x$ discrepancies rapidly increase. Likely higher order analytic corrections are the main reason for this behaviour. However also other types of corrections like $t^{\nu\omega'}$ with $\omega' \approx 1.8$ [30] should be taken into account. Therefore we abstain from fitting with $t^2$ corrections.

### 6 The specific heat of thin films of $^4$He and the thermodynamic Casimir force

In a number of experiments the excess specific heat of thin films of $^4$He and $^3$He-$^4$He mixtures has been measured in the neighbourhood of the $\lambda$-transition [11]. In these works the scaling function $f_2$ which is defined by

$$C_{bulk}(t) - C(L_0, t) \simeq L_0^{\alpha/\nu} f_2(tL_0^{1/\nu})$$

is extracted from experimental data for the specific heat of the three-dimensional bulk system $C_{bulk}(t)$ and of thin films $C(L_0, t)$, where $L_0$ is the thickness of the film. Since the specific heat is the derivative of the energy density with respect to the temperature, $f_2(x)$ is, up to a constant factor, equal to $h''(x)$. 

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Figure 5: We plot finite size scaling function $\theta$ of the thermodynamic Casimir force. We have computed $\theta$ from the finite size scaling function $h'$ of the excess energy per area of the film. For comparison we give the result of our previous work [20] where we have computed $\theta$ directly from the thermodynamic Casimir force. For a discussion see the text.
Figure 6: Similar to the previous figure. Here we have taken into account analytic correction computing the scaling function $h'$. For a discussion see the text.
To compute this factor let us start from the excess reduced free energy density:

\[ f(t, L_0) - f_{bulk}(t) \simeq L_0^{-3} h(x) \]  

(31)

where \( t = T/T_{\lambda} - 1 \) and \( x = t[L_0/\xi_0]^{1/\nu} \). Note that here, as long as the free energy density and \( L_0^{-3} \) are measured in the same units, \( h(x) \) is uniquely defined; there is no ambiguous factor.

The excess energy density is given by the derivative with respect to \( \beta = 1/(k_B T) \).

Hence

\[ E(t, L_0) - E_{bulk}(t) = -L_0^{-3}[L_0/\xi_0]^{1/\nu} \frac{1}{k_B T_{\lambda}} \beta^{-2} \simeq -L_0^{3}[L_0/\xi_0]^{1/\nu} k_B T_{\lambda} \]  

(32)

where we have approximated \( \beta^{-2} \simeq k_B^2 T_{\lambda}^2 \) in the neighbourhood of the \( \lambda \)-transition.

The specific heat as defined in the experiments is given by the derivative of the energy density with respect to the temperature. Hence

\[ C_{bulk}(t) - C(t, L_0) \simeq k_B L_0^{-3}[L_0/\xi_0]^{2/\nu} h''(x) . \]  

(33)

The results for the specific heat of the experiment are given in J mol\(^{-1} \) K\(^{-1} \). These we convert into \( k_B A^{-3} \) to get the same units on both sides of equation (33).

Note that the thickness of the films in [16, 17] is quoted in \( \AA \). To this end we need the density \( \rho_{\lambda} = 146.1087 \text{ kg/m}^3 \) of \(^4\text{He} \) at the \( \lambda \)-transition, the molar weight 4.0026... g mol\(^{-1} \) of \(^4\text{He} \) and the Boltzmann constant \( k_B = 1.38065 \ldots \times 10^{-23} \text{ JK}^{-1} \).

This amounts to the factor 0.00264... J\(^{-1} \) mol\(^{-1} \) K\(^{-1} \) A\(^{-3} \). In [32] the data are given as a function of the reduced temperature \( t = 1 - T/T_{\lambda} \), where \( T_{\lambda} = 2.17 \ldots \text{K} \). In order to plot them as a function of \( x = t[L_0/\xi_0]^{1/\nu} \) we have used \( \xi_0 = 1.422(5) \AA \) which we [13] have computed from the amplitude of the bulk specific heat of \(^4\text{He} \) at vapour pressure [33] and the universal amplitude ratio \( R_\alpha \) [26].

In figure 7 we have plotted

\[ [C_{bulk}(t) - C(L_0, t)] k_B^{-3} L_0^{3}[L_0/\xi_0]^{-2/\nu} \]  

(34)

as a function of \( x = t[L_0/\xi_0]^{1/\nu} \). To this end we have used the data given in [32] for the thicknesses 483, 1074, 2113, 5039, 6918 and 9869\AA.

Note that \( h''(0) \approx 3.05 \) as can be obtained from the results of section 4.3 of [15]. For \( x \gtrsim -5 \) the curves obtained from different thicknesses of the film fall reasonably well on top of each other. It has been noticed [11] that for \( x \lesssim -5 \), in particular in

\[ \text{It would be interesting to repeat the analysis for other data sets as e.g. those of [34].} \]
Figure 7: We plot $[C_{\text{bulk}}(t) - C(L_0, t)][L_0/\xi_0]^{-\alpha/\nu}$ as a function of $x = t[L_0/\xi_0]^{1/\nu}$. The data for thin films of $^4$He of thicknesses 483, 1074, 2113, 5039, 6918 and 9869 Å obtained in [16, 17] are taken from [32]. Note that at the critical point $t = 0$ the finite size scaling function assumes the value $\approx 3.05$. For a discussion see the text.
the neighbourhood of the minimum, the results obtained for different thicknesses differ by quite large factors. In [15] we have computed the specific heat and the scaling function \( f_2 \) starting from the data for the energy density discussed above. We find that for \( x \lesssim -5 \) our final result is clearly smaller than the experimental ones [16, 17].

Starting from the results for the finite size scaling function \( h''(x) \) obtained from different thicknesses we have computed the scaling function \( h'(x) \). To this end, we have applied the trapezoidal rule. Similar to the previous section, we have started the integration at \( x_0 \approx 4 \) in the high temperature phase. As starting value we have taken \( h'(x_0) = \frac{x}{2
u-1} h''(x_0) \). Again we have integrated \( h'(x) \) using the trapezoidal rule to get \( h(x) \). Here we have taken the same value for \( x_0 \) as above and \( h(x_0) = \frac{\nu}{2
u} h'(x_0) \). Using these results for \( h'(x) \) and \( h(x) \) we have computed \( \theta(x) \) which we have plotted in figure 8.

In order to check the effect of errors due to the finite step-size of the integration, we have repeated the integration, skipping every second value of \( x \). In order to check the effect of the singularity of \( h'(x) \) we have fitted the data for the specific heat in the neighbourhood of the transition with the ansatz

\[
h''(x) = 3.05 + c_{\pm}|x|^{-\alpha}
\]  

Then we have integrated the ansatz in the neighbourhood of the transition and compared it with the corresponding result from the trapezoidal rule. We find that the numerical results only change little and the conclusions drawn below are not effected.

Let us now discuss the results that we have obtained: For 483Å the curve is monotonically decreasing with decreasing \( x \); in particular no minimum of the function can be observed. For 1074Å a shallow minimum occurs at \( x \approx -5.3 \); for \( x \lesssim 6.1 \) the function is decreasing again with decreasing \( x \). For 2113Å we see a clear minimum at \( x \approx -5.5 \); However the value of the minimum is clearly smaller than the one of \([20]\). In the case of 5039Å and 6918Å we find a quite good match with our result \([20]\) down to \( x \approx -7 \). For 6918Å the minimum is located at \( x \approx -4.8 \) and the value of the minimum is \( \theta \approx -1.3 \). For 6918Å the minimum occurs at \( x \approx 4.65 \) and the value of the minimum is \( \theta \approx -1.36 \). For 5039Å no data for \( x < -7 \) are available. For 6918Å the curve is decreasing again for \( x \lesssim -6.7 \) with decreasing \( x \). Up to here the expectation that with increasing thickness of the film the result converges toward the universal scaling function is fulfilled. However for the largest thicknesses studied, 9869Å even the worst mismatch is found. The curve is monotonically decreasing with decreasing \( x \) and even for \( x \gtrsim 5 \) there is
Figure 8: We plot results for the scaling function $\theta$ of the thermal Casimir force. These results were obtained by numerically integrating experimental data [16, 17, 32] for the excess specific heat of thin films of $^4$He near the $\lambda$-transition. For comparison we give the result obtained in [20]. For a discussion see the text.
quite large mismatch with our result for $\theta$ [20]. Playing around with the data, one finds that smaller values of $h''(x)$ for $x \lesssim -5$ are needed to avoid that $\theta$ is decreasing with decreasing $x$ for $x \lesssim -5$. One should note that eq. (8) only holds for the scaling limit. Therefore the observations made here are not an indication that the experimental data are effected by an error. They can also be explained by corrections to the scaling behaviour. This is at least true for the smaller thicknesses like 483 Å. The result for 9869 Å is more puzzling. One should note that the analysis presented in this section does not depend on the type of boundary conditions that is realized in the experiment. But we think that the behaviour of $\theta(x)$ for $x \lesssim -5$ obtained here can not be explained by different boundary conditions from those used in the study of the lattice model [15, 20].

7 Summary and Conclusions

We have studied the relation of the excess specific heat, the excess energy and the thermodynamic Casimir force in thin films in the three-dimensional XY universality class. To this end we have exploited the relation (8)

$$\theta(x) = 2h(x) - \frac{x}{\nu} h'(x)$$

among the finite size scaling functions $\theta(x)$ of the thermodynamic Casimir force, $h(x)$ of the excess free energy and $h'(x)$ of the excess energy. We have analysed data obtained for the energy density of the improved two-component $\phi^4$ model on the simple cubic lattice and experimental results for the specific heat of thin films of $^4$He near the $\lambda$-transition [16, 17].

As a first exercise we have computed the functions $h'(x)$ and $h(x)$ for a finite lattice of the size $L^3$ with periodic boundary conditions in all directions. This way we avoid potential problems related with the Kosterlitz-Thouless phase transition of the thin film and corrections caused by Dirichlet boundary conditions. Indeed we find a good collapse of the data already for rather small lattice sizes $L = 8, 16$ and 32.

Next we have repeated the same exercise for films with free boundary conditions using the data for the excess energy density obtained in [15]. Here we find a huge mismatch between the thicknesses $L_0 = 8, 16$ and 32. Replacing $L_0$ by $L_{0,\text{eff}} = L_0 + L_s$ with $L_s = 1.02(7)$ [19] does not remove this discrepancy. We argue that the non-singular part of the energy density suffers from boundary corrections that are not described by the same $L_s$ which accounts for the corrections in singular
quantities. Indeed, the analysis of the energy density of films up to the thickness \( L_0 = 64 \) at the critical temperature of the three dimensional system results in a \( L_{\text{sns}} \) for the analytic background of the energy density that is clearly different from \( L_s \). Taking into account this result we find a reasonable collapse of the functions obtained from \( L_0 = 8, 16 \) and 32 in a large range of the scaling variable \( x \).

Computing the Casimir force from this result for \( h'(x) \) we find a good collapse for \(-7 \lesssim x < 4\). In this range of \( x \) we also find a good agreement with the result for \( \theta \) that we have obtained in [20]. Note that in particular the minimum of the scaling function \( \theta \) is within this range. We confirm the position \( x_{\text{min}} \) and the value \( \theta_{\text{min}} \) that we have obtained in [20]. Next we took into account analytic corrects. The coefficients of these corrections were computed by matching the results obtained from \( L_0 = 16 \) and \( L_0 = 32 \). This way we could extend the range of agreement with our previous result [20] down to \( x \approx -15 \).

We have presented a viable alternative to compute the scaling function \( \theta \) of the Casimir force. The nice agreement with our previous result [20] gives us further confidence in the correctness of the results.

Finally we have computed the scaling function \( \theta \) using experimental results for the excess specific heat \([16, 17]\). Here we find a reasonable match with the theoretical results in the range \( x \gtrsim -5 \). In particular we find evidence that the minimum of the scaling function \( \theta \) is located at \( x_{\text{min}} \approx 5 \) which is consistent with our prediction [20] but slightly larger than \( x_{\text{min}} = -5.45(12) \) [12] and \( x_{\text{min}} = -5.7(5) \) [13], where the thermodynamic Casimir force has been determined for films of \(^4\text{He} \) with thicknesses \( \lesssim 600\text{A} \).

In the range \( x \lesssim -5 \) the curves obtained from different thicknesses show quite different behaviour. Furthermore in this range \( \theta(x) \) is decreasing with decreasing \( x \). This behaviour corresponds to too large values of \( h''(x) \) in the range \( x \lesssim -5 \). We think that understanding this problem requires a detailed knowledge of the experiments and is therefore beyond the scope of the present work.

8 Acknowledgements

This work was supported by the DFG under the grant No HA 3150/2-1.
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