The thermodynamic Casimir effect in the neighbourhood of the $\lambda$-transition: a Monte Carlo study of an improved three-dimensional lattice model

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Abstract. We study the thermodynamic Casimir effect in thin films in the three-dimensional $XY$ universality class. To this end, we simulate the improved two-component $\phi^4$ model on the simple cubic lattice. We use lattices up to the thickness $L_0 = 33$. On the basis of the results of our Monte Carlo simulations we compute the universal finite size scaling function $\theta$ that characterizes the behaviour of the thermodynamic Casimir force in the neighbourhood of the critical point. We confirm that leading corrections to the universal finite size scaling behaviour due to free boundary conditions can be expressed using an effective thickness $L_{0,\text{eff}} = L_0 + L_s$, with $L_s = 1.02(7)$. Our results are compared with experiments on films of $^4$He near the $\lambda$-transition, previous Monte Carlo simulations of the $XY$ model on the simple cubic lattice and field-theoretic results. Our result for the finite size scaling function $\theta$ is essentially consistent with the experiments on films of $^4$He and the previous Monte Carlo simulations.

Keywords: classical Monte Carlo simulations, classical phase transitions (theory), finite-size scaling, surface effects (theory)

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1. Introduction

In 1978 Fisher and de Gennes [1] realized that when thermal fluctuations of a system are restricted by a container a force acts on its walls. Since this effect is similar to the Casimir effect, where the restriction of quantum fluctuations induces a force, it is called the ‘thermodynamic’ Casimir effect. In the last few years there has been great progress in the experimental verification of this effect and quantitative predictions for the force were obtained from Monte Carlo simulations of spin models [2].

Thermal fluctuations extend to large scales only in the neighbourhood of critical points. Hence the thermodynamic Casimir effect can only be observed in the neighbourhood of a continuous phase transition. Therefore it is also called the critical Casimir effect. Before discussing in more detail the thermodynamic Casimir effect let us recall some basic facts about critical phenomena and the implications of restricting geometries in the neighbourhood of critical points. In the neighbourhood of the critical point, various quantities diverge in the thermodynamic limit following power laws. For example the correlation length, which measures the spatial extent of fluctuations, behaves as

\[ \xi \simeq \xi_{0,\pm}|t|^{-\nu} \]  

where \( t = (T - T_c)/T_c \) is the reduced temperature and \( T_c \) the critical temperature. \( \xi_{0,+} \) and \( \xi_{0,-} \) are the amplitudes of the correlation length in the high and low temperature phases, respectively. While \( \xi_{0,+} \) and \( \xi_{0,-} \) depend on the microscopic details of the system, the critical exponent \( \nu \) and the ratio \( \xi_{0,+}/\xi_{0,-} \) are universal. This means that they assume exactly the same values for all systems within a given universality class. A universality class is characterized by the spatial dimension of the system, the range of the interaction and the symmetry of the order parameter. The modern theory of critical phenomena is the renormalization group (RG). For reviews see e.g. [3]–[6]. Here we consider the XY
universality class in three dimensions with short range interactions. This universality class is of particular interest, since the \( \lambda \)-transition of \(^4\)He is supposed to share this universality class. The most accurate experimental results for critical exponents and universal amplitude ratios for a three-dimensional system have been obtained for this transition; for a review see \cite{7}.

The effect of a confining geometry becomes noticeable when the correlation length \( \xi \) is of similar size to or larger than the linear extent \( L_0 \) of the system. If the system is finite in all directions, thermodynamic functions have to be analytic. Hence a singular behaviour like that of equation (1) is excluded. As a remnant of the singularities there remain peaks in the neighbourhood of the transition. With increasing linear extent \( L_0 \) the heights of these peaks increase and the temperatures of the maxima approach the critical temperature. This behaviour is described by the theory of finite size scaling (FSS); for reviews see \cite{8, 9, 10}. The essence of finite size scaling is that the physics of a finite system in the neighbourhood of a critical point is governed by the ratio \( L_0/\xi \), where \( L_0 \) is the linear extent of the container and \( \xi \) the correlation length of the bulk system. Furthermore it depends on the geometry of the container and on the type of the boundary conditions that the container imposes on the order parameter.

Thin films are finite in one direction and infinite in the other two directions. Hence singular behaviour is still possible; however the associated phase transition belongs to a two-dimensional universality class. Therefore in the case of O(2) symmetry that we consider here, a Kosterlitz-Thouless (KT) transition \cite{11–13} is expected. In \cite{14} we have studied lattice models with O(2) symmetry and thin film geometry. We have confirmed the KT nature of the transition and have studied the scaling of the transition temperature with the thickness of the film. Up to scaling corrections, the KT transition occurs, as predicted by finite size scaling theory, at a particular value of \( L_0/\xi \). In \cite{14} we find \( [L_0/\xi_T]_{KT} = 1.595(7) \) where \( \xi_T \) is the transverse correlation length which is defined in the low temperature phase of the bulk system. Using equation (1) this result can be rewritten as \( t_{KT}[L_0/\xi_T,0]^{1/\nu} = -2.004(13) \), where \( t_{KT} = (T_{KT} - T_c)/T_c \) and \( \nu = 0.6717(1) \) \cite{25}. Hence the transition temperature \( T_{KT} \) of the film approaches the critical temperature \( T_c \) of the three-dimensional bulk system as the thickness \( L_0 \) increases. In the following, for consistency with the literature, we shall set the scale by using the correlation length in the high temperature phase. Correspondingly, by using equation (52) of \cite{14} we find\(^2\)

\[
t_{KT}[L_0/\xi_0]^{1/\nu} = -7.48(3).
\]

Now let us turn again to the thermodynamic Casimir effect. 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 and \( \tilde{f}_\text{ex} = \tilde{f}_\text{film} - L_0\tilde{f}_\text{3D} \) is the excess free energy per area of the film, where \( \tilde{f}_\text{film} \) is the free energy per area of the film and \( \tilde{f}_\text{3D} \) the free energy density of the thermodynamic limit of the three-dimensional system; see e.g. \cite{15}. Finite

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\(^1\) For a review on experimental studies of \(^4\)He near the \( \lambda \)-transition in confining geometries see \cite{10}.

\(^2\) Since in the following we shall only use the amplitude of the correlation length in the high temperature phase, we have omitted the subscript + in \( \xi_0 \).
size scaling predicts that the Casimir force behaves as

\[ F_{\text{Casimir}} = \frac{k_B T}{L_0^3} \theta\left(t\left[\frac{L_0}{\xi_0}\right]^{1/\nu}\right) \]  

where \( \theta(x) \) is a universal finite size scaling function. In [16,17] \(^4\)He films of a thickness up to \( \approx 600 \) Å on a substrate have been studied. The Casimir force is deduced from the thinning of the films in the neighbourhood of the \( \lambda \)-transition. Since the films are thinning, the force is negative. The authors demonstrate that their data for the Casimir force are consistent with the finite size scaling ansatz (4). The Casimir force displays a pronounced minimum at \( x = t\left(\frac{L_0}{\xi_0}\right)^{1/\nu} \approx -5.5 \).

It has been a challenge for theorists to compute the finite size scaling function \( \theta(x) \). Krech and Dietrich [18,19] have computed it in the high temperature phase using the \( \epsilon \)-expansion up to \( O(\epsilon) \). This result is indeed consistent with the measurements on \(^4\)He films. Deep in the low temperature phase, the spin wave approximation should provide an exact result. It predicts a negative non-vanishing value for \( \theta(x) \). However the experiments suggest a much larger absolute value for \( \theta(x) \) in this region. Until recently a reliable theoretical prediction for the minimum of \( \theta(x) \) and its neighbourhood was missing. Using a renormalized mean field approach the authors of [20,21] have computed \( \theta(x) \) for the whole temperature range. Qualitatively they reproduce the features of the experimental result. However the position of the minimum is by almost a factor of 2 different from the experimental one. The value at the minimum is wrongly estimated by a factor of about 5.

Only quite recently Monte Carlo simulations of the XY model on the simple cubic lattice [22]–[24] provided results for \( \theta(x) \) which essentially reproduce the experiments on \(^4\)He films [16,17]. These simulations were performed with lattices of a thickness up to \( L_0 = 16 \) [23] and up to \( L_0 = 20 \) [24]. The authors of [24] pointed out that for these lattice sizes corrections to scaling still play an important role. The purpose of the present work is to get accurate control over the leading corrections to scaling, allowing us to compute \( \theta(x) \) with reliable error bars.

As the first step in this direction we simulate the improved two-component \( \phi^4 \) model instead of the XY model. For a precise definition of these models see the section below. In this way we avoid leading corrections to scaling which are \( \propto L_0^{-\omega} \) with \( \omega = 0.785(20) \) [25]; similar values for the exponent are obtained with field-theoretic methods; for a review see e.g. [6]. In order to mimic the vanishing order parameter that is observed at the boundaries of \(^4\)He films, Dirichlet boundary conditions with vanishing field are imposed. These lead to corrections \( \propto L_0^{-1} \) [26], which can be eliminated by replacing the thickness \( L_0 \) by an effective one \( L_{0,\text{eff}} = L_0 + L_s \), where \( L_s = 1.02(7) \) [14] for the model that we have simulated\(^3\).

This paper is organized as follows. First we define the model and the observables that we have measured. Next we discuss the finite size scaling behaviour of the Casimir force. In particular, we discuss corrections to scaling caused by the Dirichlet boundary conditions. We outline the method used to compute the Casimir force. We discuss the simulations that have been performed and analyse our data. We compare our

\(^3\) In the literature, replacing \( L_0 \) by \( L_{0,\text{eff}} = L_0 + L_s \) to account for surface corrections was first discussed by Capehart and Fisher [27] in the context of the surface susceptibility of Ising films.
results with experiments [16, 17], previous Monte Carlo simulations [23, 24] and the $\epsilon$-expansion [18, 19]. 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 with $x = (x_0, x_1, x_2)$. The components of $x$ might assume the values $x_i \in \{1, 2, \ldots, L_i\}$. We simulate lattices of the size $L_1 = L_2 = L$ and $L_0 \ll L$. In the 1-direction and the 2-direction we employ periodic boundary conditions and free boundary conditions in the 0-direction. This means that the sites with $x_0 = 1$ and $x_0 = L_0$ have only five nearest neighbours. This type of boundary condition could be interpreted as Dirichlet boundary conditions with 0 as the value of the field at $x_0 = 0$ and $x_0 = L_0 + 1$. Note that viewing 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 [14] and might be a good starting point for a field-theoretic calculation of $L_s$. The Hamiltonian of the two-component $\phi^4$ model, for a vanishing external field, is given by

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

(5)

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

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

(6)

Note that following the conventions of our previous work, e.g. [29], we have absorbed the inverse temperature $\beta$ into the Hamiltonian$^4$. In the limit $\lambda \to \infty$ the field variables are fixed to unit length; hence 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 $\lambda^* = 2.10(6)$ [28], $\lambda^* = 2.07(5)$ [29] and most recently $\lambda^* = 2.15(5)$ [25]. The inverse of the critical temperature $\beta_c$ has been determined accurately for several values of $\lambda$ using finite size scaling (FSS) [25]. 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 [14, 25, 31, 32]. At $\lambda = 2.1$ one gets $\beta_c = 0.5091503(6)$ [25]. 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 [25], it should be by at least a factor 20 smaller than for the standard $XY$ model.

The second moment correlation function is defined by

$$\xi_{2nd}^2 = \frac{\mu_2}{2d\mu_0}$$

(7)

$^4$ Therefore, following [5] we actually should call it the reduced Hamiltonian.
where \( d = 3 \) is the dimension of the system, and \( \mu_i = \sum_x |x|^i \langle \vec{\phi}_0 \cdot \vec{\phi}_x \rangle_c \) where \( \langle \vec{\phi}_0 \cdot \vec{\phi}_x \rangle_c \) is the connected two-point correlation function at the distance \( x = (x_0, x_1, x_2) \). In [14] we find for \( \lambda = 2.1 \) by fitting our data

\[
\xi_{2nd} = 0.26362(8)t^{-0.6717} \times [1 + 0.039(8)t^{0.527} - 0.72(4)t]
\]  

(8)

where \( t = 0.5091503 - \beta \).\(^5\) Throughout we use \( \nu = 0.6717(1) \) [25] as the value of the critical exponent of the correlation length. Recent experiments on the \( \lambda \)-transition of \(^4\)He suggest a slightly smaller value: \( \nu = 0.6709(1) \) [33]. This discrepancy is however not crucial for the present study. Note that in the high temperature phase there is only a little difference between \( \xi_{2nd} \) and the exponential correlation length \( \xi_{exp} \) which is defined by the asymptotic decay of the two-point correlation function. Following [29],

\[
\lim_{t \to 0} \frac{\xi_{exp}}{\xi_{2nd}} = 1.000204(3) \quad (t > 0)
\]  

(9)

for the thermodynamic limit of the three-dimensional system. Hence at the level of precision reached here it does not matter whether \( \xi_{0,exp} \) 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

\[
f = -\frac{1}{L_0L_1L_2} \log Z.
\]  

(10)

That is, compared with the free energy density \( \tilde{f} \), a factor \( k_B T \) is skipped.

Note that in equation (5) \( \beta \) 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 [30], we multiply by \(-1\):

\[
E = \frac{1}{L_0L_1L_2} \frac{\partial \log Z}{\partial \beta}.
\]  

(11)

It follows that

\[
E = \frac{1}{L_0L_1L_2} \left\langle \sum_{(x,y)} \vec{\phi}_x \cdot \vec{\phi}_y \right\rangle,
\]  

(12)

which can be easily determined in Monte Carlo simulations. From equations (10) and (11) it follows that the free energy density can be computed as

\[
f(\beta) = f(\beta_0) - \int_{\beta_0}^{\beta} d\tilde{\beta} E(\tilde{\beta}).
\]  

(13)

\(^5\) We shall use this definition of the reduced temperature also in the following discussion of our numerical results; hence \( \xi_{0} = 0.26362(8) \).
3. The finite size scaling behaviour of the thermal Casimir force

Let us discuss the scaling behaviour of the reduced excess free energy. 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 into singular (s) and non-singular (ns) parts:

$$f_{\text{ex}}(t, L_0) = f_{\text{film}}(t, L_0) - L_0 f_{3D}(t) = f_{\text{film},s}(t, L_0) + L_{0,\text{eff},\text{ns}} f_{\text{ns}}(t) - L_0 f_{3D,s}(t) - L_0 f_{\text{ns}}(t)$$

$$= L_{0,\text{eff}}^{-2} h(x) + L_s f_{3D,s}(t) + L_{\text{ns}} f_{\text{ns}}(t)$$  \hspace{1cm} (14)

where $h(x) = L_{0,\text{eff}}^2 [f_{\text{film},s}(t, L_0) - L_{0,\text{eff}} f_{3D,s}(t)]$ 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 \textit{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 [15]

$$\beta F_{\text{Casimir}} = -\frac{\partial f_{\text{ex}}(t, L_0)}{\partial L_0} = 2 L_{0,\text{eff}}^{-3} h(x) - L_{0,\text{eff}}^{-3} \frac{1}{\nu} x h'(x) = L_{0,\text{eff}}^{-3} \theta(x)$$  \hspace{1cm} (15)

where $\theta(x) = 2h(x) - (x/\nu)h'(x)$.

4. Computing the Casimir force on the lattice

Here we follow essentially the approach of [23]. For an alternative method see [22, 24]. On the lattice the thickness $L_0$ assumes integer values. Therefore we approximate the derivative for half-integer values of $L_0$ as

$$\frac{\partial f_{\text{ex}}(\beta, L)}{\partial L} \bigg|_{L=L_0} \approx \Delta f_{\text{ex}}(\beta, L_0) = f(\beta, L_0 + 1/2) - f(\beta, L_0 - 1/2) + f_{3D}(\beta).$$  \hspace{1cm} (16)

Correspondingly we define

$$\Delta E_{\text{ex}}(\beta, L_0) = E(\beta, L_0 + 1/2) - E(\beta, L_0 - 1/2) - E_{3D}(\beta)$$  \hspace{1cm} (17)

where $E(\beta, L_0)$ is the energy per area of a thin film and $E_{3D}(\beta)$ the energy density of the three-dimensional system. By analogy with equation (13) we compute

$$\Delta f_{\text{ex}}(\beta) = -\int_{\beta_0}^{\beta} d\tilde{\beta} \Delta E_{\text{ex}}(\tilde{\beta})$$  \hspace{1cm} (18)

where $\beta_0$ is chosen such that $\xi(\beta_0) \ll L_0$ and hence the Casimir force vanishes.

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Table 1. We characterize our new simulations. In the first column we give the thickness $L_0$ of the film. In the second column we give the linear size $L = L_1 = L_2$ of the lattice in the other two directions. In the third and fourth columns we give the upper and lower bounds of the interval in $\beta$ that has been simulated. In the fifth column we give the step size $\Delta \beta$ that we used. For example $\beta_{\text{min}} = 0.49$, $\beta_{\text{max}} = 0.519$ and $\Delta \beta = 0.001$ mean that $\beta = 0.49, 0.491, 0.492, \ldots, 0.519$ have been simulated. Finally, in the last column we give the number of measurements (stat) that we have performed for each of the simulations.

| $L_0$ | $L_1 = L_2$ | $\beta_{\text{min}}$ | $\beta_{\text{max}}$ | $\Delta \beta$ | Stat |
|-------|-------------|----------------------|----------------------|---------------|------|
| 9     | 64          | 0.49                 | 0.519                | 0.001         | $5 \times 10^5$ |
| 9     | 128         | 0.52                 | 0.527                | 0.001         | $2 \times 10^5$ |
| 9     | 256         | 0.528                | 0.56                 | 0.001         | $10^5$ |
| 9     | 256         | 0.562                | 0.58                 | 0.002         | $10^5$ |
| 9     | 512         | 0.536                | 0.539                | 0.001         | $10^5$ |
| 9     | 512         | 0.5395               | 0.548                | 0.0005        | $10^5$ |
| 9     | 512         | 0.548                | 0.57                 | 0.001         | $10^5$ |
| 9     | 1024        | 0.539                | 0.548                | 0.0005        | $10^5$ |
| 17    | 256         | 0.527                | 0.55                 | 0.001         | $2 \times 10^5$ |
| 17    | 512         | 0.5                  | 0.512                | 0.001         | $10^5$ |
| 17    | 512         | 0.5125               | 0.529                | 0.0005        | $10^5$ |
| 17    | 512         | 0.53                  | 0.55                 | 0.001         | $10^5$ |
| 17    | 1024        | 0.5205               | 0.529                | 0.0005        | $8 \times 10^4$ |
| 33    | 256         | 0.502                | 0.50875              | 0.00025       | $4 \times 10^5$ |
| 33    | 512         | 0.509                | 0.5128               | 0.0002        | $3 \times 10^5$ |
| 33    | 1024        | 0.513                |                      |               | $10^5$ |
| 33    | 1024        | 0.5132               |                      |               | $8 \times 10^4$ |

5. Numerical results

In [30] we have studied the specific heat of thin films in the two-component $\phi^4$ model at $\lambda = 2.1$. To this end, we had determined the energy density for the three-dimensional thermodynamic limit and for films of the thicknesses $L_0 = 8, 16$ and 32 for a large number of $\beta$-values. In order to compute the derivative with respect to $L_0$, we have complemented these simulations with ones for $L_0 = 9, 17$ and 33. The Monte Carlo algorithm that has been used is the same as in [30]: an update cycle is composed of a Metropolis sweep, a few overrelaxation sweeps and single-cluster [34] and wall cluster [35] updates. One sweep means that a local update is performed at each site of the lattice once. As the random number generator we have used the SIMD-oriented Fast Mersenne Twister algorithm [36]. In table 1 we have summarized the statistics of our runs. In total, these simulations took about three years of CPU time on a single core of a Quad-Core Opteron(tm) 2378 CPU (2.4 GHz).

Using these data, we have computed $\Delta E_{\text{ex}}$ for $L_0 = 8.5, 16.5$ and 32.5. One should note that the statistical error of $E(\beta, L_0 + 1/2) - E(\beta, L_0 - 1/2)$ is much larger than that of $E_{\text{3D}}(\beta)$. In order to obtain $\Delta f_{\text{ex}}$ we have numerically integrated $\Delta E_{\text{ex}}$ using the trapezoidal rule:

$$-\Delta f_{\text{ex}}(\beta_n) \approx \sum_{i=0}^{n-1} \frac{1}{2} (\beta_{i+1} - \beta_i) (\Delta E_{\text{ex}}(\beta_{i+1}) + \Delta E_{\text{ex}}(\beta_i))$$  \hspace{1cm} (19)
where $\beta_i$ are the values of $\beta$ that we have simulated at. They are ordered such that $\beta_{i+1} > \beta_i$ for all $i$. We have chosen $\beta_0 = 0.49, 0.5$ and $0.505$ for $L_0 = 8.5, 16.5$ and $32.5$. We find that $\Delta E_{ext}$ is equal to zero within error bars up to values of $\beta$ that are slightly larger than the $\beta_0$ that we have chosen.

The estimate obtained from the integration is affected by statistical and systematical errors. The statistical one can be easily computed, since the $\Delta E_{ext}$ are obtained from independent simulations:

$$
\epsilon^2(-\Delta f_{ext}(\beta_n)) = \frac{(\beta_1 - \beta_0)^2}{4} \epsilon^2[\Delta E_{ext}(\beta_0)] + \frac{(\beta_n - \beta_{n-1})^2}{4} \epsilon^2[\Delta E_{ext}(\beta_n)]
$$

$$
+ \sum_{i=1}^{n-1} \frac{(\beta_{i+1} - \beta_{i-1})^2}{4} \epsilon^2[\Delta E_{ext}(\beta_i)]
$$

(20)

where $\epsilon^2$ denotes the square of the statistical error.

In order to estimate the error due to the finite step size $\beta_{i+1} - \beta_i$ we have redone the integration, skipping every second value of $\beta$, i.e. doubling the step size. In all three cases (i.e. $L_0 = 8.5, 16.5$ and $32.5$), the results were consistent within the statistical errors. Therefore we are confident that the systematical error due to the finite step size is smaller than the statistical one.

In the upper part of figure 1 we have plotted $-L_0^3 \Delta f_{ext}$ as a function of $-t[L_0/\xi_0]^{1/\nu}$, where we have used $\nu = 0.6717$ and $\xi_0 = 0.26362$, equation (8). We find that throughout, the function assumes a negative value. In all cases it has a single minimum at $t[L_0/\xi_0]^{1/\nu} \approx -5$.

The position of the minimum $\beta_{\text{min}}(L_0)$ can be easily determined: it is given by the zero of $\Delta E_{ext}$. We have computed $\beta_{\text{min}}(L_0)$ by linearly fitting $\Delta E_{ext}$ in the neighbourhood of the minimum. In addition to performing simulations $L_0 = 8.5, 16.5$ and $32.5$ we performed ones for $L_0 = 6.5, 7.5, 9.5, 12.5$ and $24.5$ at a few values of $\beta$ in the neighbourhood of $\beta_{\text{min}}$. Our results are summarized in table 2.

The curves for $L_0 = 8.5, 16.5$ and $32.5$ plotted in figure 1 do not fall on top of each other. In particular, both the position and the value of the minimum are quite different for different $L_0$. In order to take corrections into account we have replaced $L_0$ by $L_{0,\text{eff}} = L_0 + L_s$, where $L_s = 1.02(7)$ [14]. To this end, in the lower part of figure 1 we have plotted $-L_{0,\text{eff}}^3 \Delta f_{ext}$ as a function of $-t[L_{0,\text{eff}}/\xi_0]^{1/\nu}$, where we have used the central value of the shift $L_s = 1.02$. Now the distance between the curves for different $L_0$ is indeed much reduced compared with the case for the upper part of figure 1. The results for $L_0 = 16.5$ and $L_0 = 32.5$ are almost consistent within error bars. Note that using $L_s = 0.95$ the matching of the data for different $L_0$ seems to be better than for $L_s = 1.02$.

Let us discuss in more detail the results obtained for the minimum of the finite size scaling function $\theta(x)$. Using the numbers given in the third column of table 2 and $L_s = 1.02$ we get $-\Delta f_{ext,\text{min}}L_{0,\text{eff}}^3 = -1.365(3), -1.341(6)$ and $-1.311(19)$ for $L_0 = 8.5, 16.5$ and $32.5$, respectively. Using instead $L_s = 0.95$ we get $-1.335(3), -1.325(6)$ and $-1.302(19)$ for $L_0 = 8.5, 16.5$ and $32.5$, respectively. As our final result we take the one obtained from $L_0 = 32.5$ and $L_s = 1.02$:

$$
\theta_{\text{min}} = -1.31(3),
$$

(21)

where the error that is quoted takes into account the statistical error and the uncertainty of $L_s$. 

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Next we fitted our results for $\beta_{\text{min}}$ with the ansatz

$$t_{\text{min}}(1 + ct_{\text{min}})(L_{0,\text{eff}}/\xi_0)^{1/\nu} = x_{\text{min}}$$

(22)

where $t_{\text{min}} = \beta_c - \beta_{\text{min}}$. We have used $\nu = 0.6717$, $\xi_0 = 0.26362$, $\beta_c = 0.5091503$ and $L_s = 1.02$ as the input and $c$ and $x_{\text{min}}$ as parameters of the fit. The term $(1 + ct_{\text{min}})$ parametrizes analytic corrections. We did not include a correction with the exponent $\theta' \approx 1.2$ [37], since within the accuracy of our data they cannot be discriminated from the leading analytic correction. The results of these fits are summarized in table 3. The $\chi^2$/d.o.f. is reasonably small starting from $L_{0,\text{min}} = 6.5$, where all thicknesses $L_0$ with
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Table 2. We give the position $\beta_{\text{min}}$ of the minimum of the Casimir force and its value $-\Delta f_{\text{ex, min}}$ as a function of the thickness $L_0$.

| $L_0$ | $\beta_{\text{min}}$ | $-\Delta f_{\text{ex, min}}$ |
|-------|----------------------|-----------------------------|
| 6.5   | 0.54432(2)           |                            |
| 7.5   | 0.53814(2)           |                            |
| 8.5   | 0.53354(2)           | -0.001582(3)               |
| 9.5   | 0.53010(2)           |                            |
| 12.5  | 0.52348(2)           |                            |
| 16.5  | 0.51886(2)           | -0.0002494(11)             |
| 24.5  | 0.51463(2)           |                            |
| 32.5  | 0.51279(2)           | -0.0000348(5)              |

Table 3. We fit our results for $\beta_{\text{min}}$ with ansatz (22). $L_{0, \text{min}}$ is the smallest thickness of the film that is included into the fit.

| $L_{0, \text{min}}$ | $x_{\text{min}}$ | $c$ | $\chi^2$/d.o.f. |
|---------------------|------------------|-----|-----------------|
| 6.5                 | -4.942(6)        | 1.20(4) | 1.47            |
| 7.5                 | -4.945(8)        | 1.17(7) | 1.72            |
| 8.5                 | -4.956(10)       | 1.04(10) | 1.32           |
| 9.5                 | -4.952(12)       | 1.10(12) | 1.64           |

$L_0 \geq L_{0, \text{min}}$ are included in the fit. Also the estimates for $x_{\text{min}}$ and $c$ do not change much as $L_{0, \text{min}}$ is changed. In order to check the dependence of the results on the value of $L_s$ we have repeated the fit for $L_{0, \text{min}} = 8.5$ using $L_s = 0.95$ instead of $L_s = 1.02$. We get the $x_{\text{min}} = -4.943(10)$, $c = 0.70(10)$ with $\chi^2$/d.o.f. = 1.12. As our final result we take

$$x_{\text{min}} = -4.95(3)$$

(23)

where the error bar covers the statistical error and the uncertainty of $L_s$. Note that the KT transition of the thin film occurs at $x_{\text{KT}} = -7.48(3)$ [14], i.e. at a considerably lower temperature. The peak of the specific heat $C$ of the thin film is located between $x_{\text{KT}}$ and $x_{\text{min}}$ at $x_C, \text{peak} = -6.4$ [30].

Our result for $x_{\text{min}}$ can be compared with those given in the literature. The experimental works [16] give $x_{\text{min}} = -5.45(12)$ (no final result for $\theta_{\text{min}}$ is quoted) and [17] $x_{\text{min}} = -5.7(5)$ and $\theta_{\text{min}} = -1.30(3)$. In [16] and [17] the convention $x = tL_0^{1/\nu}$ is used. In order to convert to $x = t[L_0/\xi_0]^{1/\nu}$ we have used $\xi_0 = 1.422\text{Å}$ for $^4\text{He}$ at the vapour pressure as discussed in section 4.2 of [30].

In his Monte Carlo study of the $XY$ model on the simple cubic lattice, Hucht [23] finds $x = -5.3(1)$ and $\theta_{\text{min}} = -1.35(3)$. The authors of [24] have used two different ansätze for the corrections to scaling. Using the first one, they arrive at $x_{\text{min}} = -5.43(2)$ and $\theta_{\text{min}} = -1.396(6)$ and using the second one, at $x_{\text{min}} = -5.43(2)$ and $\theta_{\text{min}} = -1.260(5)$.

Our result for $\theta_{\text{min}}$ is in good agreement with both the experiment [17] as well as previous Monte Carlo studies of the $XY$ model [23,24]. On the other hand, the position of the minimum $x_{\text{min}}$ differs by several times the quoted error bar from both the experiment [16,17] and from Monte Carlo studies of the $XY$ model [23,24].

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Figure 2. Here $-T_{0,\text{eff}}^3 \Delta f_{\text{ex}}$ is plotted as a function of $-t(1 + 1.04t)(L_{0,\text{eff}}/\xi_0)^{1/\nu}$ for $L_0 = 8.5, 16.5$ and $32.5$, where we use $\nu = 0.6717$, $\xi_0 = 0.26362$ and $L_{0,\text{eff}} = L_0 + L_s$ with $L_s = 1.02$. For a discussion see the text.

Finally, in figure 2 we take into account the analytic corrections that we have detected fitting the position $t_{\text{min}}$ of the minimum of the Casimir force. To this end, we have replaced the argument $t(L_{0,\text{eff}}/\xi_0)^{1/\nu}$ by $t(1 + 1.04t)(L_{0,\text{eff}}/\xi_0)^{1/\nu}$. The coefficient of the analytic correction is taken from the fit where we have fixed $L_s = 1.02$ and $L_{0,\text{min}} = 8.5$. Now we find an almost perfect match between the curves obtained from $L_0 = 8.5, 16.5$ and $32.5$.

5.1. Comparison with other theoretical approaches

Krech and Dietrich [18,19] have computed the finite size scaling function $\theta$ in the high temperature phase using the $\epsilon$-expansion up to $O(\epsilon)$. In figure 3 we plot their result for the $XY$ universality class ($N = 2$) setting $\epsilon = 1$. For comparison we plot our results for $L_0 = 8.5, 16.5$ and $32.5$. We have taken into account leading boundary corrections by replacing $L_0$ by $L_{0,\text{eff}} = L_0 + L_s$, where we have taken $L_s = 1.02$.

Comparing with the $\epsilon$-expansion we can estimate the systematical error caused by setting $\Delta f_{\text{ex}}(\beta_0) = 0$ in equation (19): we read off from the $\epsilon$-expansion that $\theta \approx -0.0035, -0.0022, -0.0015$ for our choices of $\beta_0$ for $L_0 = 8.5, 16.5$ and $32.5$. Taking into account this error, we see a good agreement of our Monte Carlo results and the $\epsilon$-expansion down to $L_0/\xi \approx 1$. The curve obtained from the $\epsilon$-expansion flattens as the critical point is approached. At the critical point the slope vanishes. In contrast, in our case, the curve steepens as the critical point is approached.

The authors of [20,21] have computed the finite size scaling function $\theta$ using a renormalized mean field approach. While this approach correctly reproduces qualitative features of the finite size scaling function $\theta$ it fails to give quantitatively accurate results. In particular one gets $x_{\text{min}} = -\pi^2 \approx -9.8696$ and $\theta_{\text{min}} \approx -6.92$. This means that the position of the minimum is overestimated by about a factor of 2 and its value by a factor of about 5.
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Figure 3. We plot the finite size scaling function $\theta$ as a function of $L_0/\xi$ in the high temperature phase obtained by Krech and Dietrich [18, 19] using the $\epsilon$-expansion. For comparison we give our results obtained for $L_0 = 8.5, 16.5$ and $32.5$. In the case of our data the leading boundary correction is taken into account by replacing $L_0$ by $L_{0,\text{eff}} = L_0 + L_s$ with $L_s = 1.02$. For a discussion see the text.

5.2. Comparison with experimental results

Finally we compare our result for the finite size scaling function $\theta$ with experiments [16, 17]. In [16] films of thicknesses between 298 and 588 Å have been studied. In figure 4 we have plotted the data obtained from capacitor 1 which corresponds to the thickness 575 Å of the film at temperatures $T > T_\lambda$. This set of data is the smoothest among the five sets given in [16, 38]. The results of [17] are, in the range of temperatures that we are interested in, less precise than those of [16]. In the tables provided by the authors [38] the finite size scaling function $\theta$ is given as a function of $(T/T_\lambda - 1)L_0^{1/\nu}$. In order to compare with our results we have converted this to $(T/T_\lambda - 1)(L_0/\xi_0)^{1/\nu}$, using $\xi_0 = 1.422$ Å. For comparison we give our result obtained from $L_0 = 16.5$, where we have taken into account the boundary correction by replacing $L_0$ by $L_{0,\text{eff}}$ and the leading analytic correction as discussed above. Furthermore, we give the asymptotic value [39, 40]

$$\lim_{x \to -\infty} \theta(x) = -\frac{\zeta(3)}{8\pi} \approx -0.04783$$

obtained from the spin wave approximation.

As already observed by the authors of [23, 24] there is a qualitative agreement between the result obtained from Monte Carlo simulations of lattice models and the experiment. There is a reasonable agreement of the position of the minimum $x_{\text{min}}$, as already discussed above. For $x < x_{\text{min}}$ our result is in good agreement with that of the experiment. In contrast, for $x > x_{\text{min}}$ the experimental value of $\theta$ is clearly smaller than ours. Actually, in this range of $x$ the discrepancy between our result and the experiments is more pronounced.

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Figure 4. We plot the finite size scaling function \( \theta(x) \) obtained from an experiment on a thin film of \( ^4 \text{He} [16,38] \), where \( x = (T/T_{\lambda} - 1)(L_0/\xi_0)^{1/\nu} \) with \( \xi_0 = 1.422 \text{ Å} \). For comparison we give our result obtained from \( L_0 = 16.5 \), where we have taken into account boundary and analytic corrections as in figure 2. Furthermore we give the asymptotic value \(-0.04783\) for \( x \to -\infty \) (dashed line). The authors of [40] have argued that fluctuations of the surface of the \( ^4 \text{He} \) film give an additional contribution to the Casimir force. The corresponding asymptotic value \(-0.1315\) is given by the dotted line. For a discussion see the text.

than in the case of [23,24]. For \( x \approx -30 \) the experimental result (capacitor 1 of [16]) assumes \( \approx -0.19 \) and is decreasing again for smaller values of \( x \). This is clearly different from the prediction (24) from the spin wave approximation.

In [40] it was argued that this discrepancy could be explained by fluctuations of the surface resulting in

\[
\lim_{x \to -\infty} \tilde{\theta}(x) = -\frac{11\zeta(3)}{32\pi} \approx -0.1315. \tag{25}
\]

This does indeed go in the right direction; it cannot however fully explain the difference between the experimental result and the theoretical prediction (24). It is an interesting question at which value of \( x \) this additional effect sets in. In particular, this effect might cause the mismatch of \( x_{\min} \) determined here and obtained from the experiments.

6. Summary and conclusions

We have studied the thermodynamic Casimir effect for thin films in the \( XY \) universality class. The behaviour of the thermodynamic Casimir force in the neighbourhood of the critical point is characterized by the universal finite size scaling function \( \theta(x) \), with \( x = t[L_0/\xi_0]^{1/\nu} \), where \( t \) is the reduced temperature, \( L_0 \) the thickness of the film, \( \xi_0 \) the amplitude of the correlation length in the high temperature phase and \( \nu \) the critical exponent of the correlation length. We have computed \( \theta \) and have compared our
As discussed in [24], corrections to scaling are numerically quite large for the thicknesses that can be studied at present. The main purpose of the present work is to get better control over these corrections. To this end, we have studied the two-component \( \phi^4 \) model on the simple cubic lattice \([22]–[24]\), field-theoretic methods \([18,19]\) and the mean field approach \([20,21]\).

In this model leading corrections to finite size scaling which are \( \propto L_0^{-\omega} \), where \( \omega = 0.785(20) \), are suppressed at least by a factor of 20 compared with the XY model ones \([25]\). In order to mimic the vanishing order parameter at the surface of \(^4\)He films near the \( \lambda \)-transition, we impose Dirichlet boundary conditions with a vanishing field. These lead to corrections \( \propto L_0^{-1} \), which can be expressed in terms of an effective thickness \( L_0,\text{eff} = L_0 + L_s \) of the film. In \([14]\) we have determined \( L_s = 1.02(7) \) for the two-component \( \phi^4 \) model at \( \lambda = 2.1 \) by using a finite size scaling study at the critical point of the three-dimensional system. We have verified that this choice of \( L_s \) does indeed eliminate the leading boundary correction in the scaling of the temperature of the Kosterlitz–Thouless transition \([14]\) and the specific heat of thin films \([30]\). Also here we confirm that corrections can be essentially eliminated by replacing \( L_0 \) by \( L_0,\text{eff} = L_0 + L_s \) with \( L_s = 1.02(7) \). The remaining discrepancies can be fitted by means of analytic corrections.

Essentially we confirm the results obtained by previous Monte Carlo simulations of the three-dimensional XY model \([23,24]\) for the finite size scaling function \( \theta \). The main discrepancy with these previous works is the position \( x_{\text{min}} = -4.95(3) \) of the minimum of \( \theta \) compared with \( x_{\text{min}} = -5.3(1) \) \([23]\) and \( x_{\text{min}} = -5.43(2) \) \([24]\).

We should note that the Monte Carlo simulation of lattice models is at the moment the only theoretical method that allows for a quantitatively accurate calculation of \( \theta \) in the low temperature phase not too far from the critical point. The \( \epsilon \)-expansion gives correctly the behaviour in the high temperature phase. The spin wave approximation gives the exact result in the limit \( x \to -\infty \). The mean field calculation of \([20,21]\) reproduces only qualitatively the features of the scaling function. Quantitatively it is not satisfactory: the position of the minimum is wrongly estimated by a factor of almost 2 and its value by a factor of about 5.

Qualitatively the Monte Carlo studies of lattice models nicely reproduce the finite size scaling function obtained from the experimental data \([16,17,38]\) for films of \(^4\)He. For \( x > x_{\text{min}} \) there is a very good quantitative agreement between the two. In contrast, for \( x < x_{\text{min}} \) the value obtained from the experiment is clearly smaller than that of the Monte Carlo studies. At large values of \( -x \) the spin wave approximation should become exact. Also in this regime, the experiments produce numbers that are too small compared with the theoretical one. The authors of \([40]\) explain this discrepancy in terms of fluctuations of the surface of the \(^4\)He film. Their result does indeed reduce but does not completely eliminate the difference between experiment and theory. Therefore it might be interesting to perform Monte Carlo simulations of a lattice model that incorporates fluctuations of the surface of the film.

Finally let us mention that the Kosterlitz–Thouless transition of the thin film occurs at \( x_{\text{KT}} = -7.48(3) \) \([14]\) which in considerably lower than \( x_{\text{min}} = -4.95(3) \). The peak of the specific heat \( C \) of the thin film is located between \( x_{\text{KT}} \) and \( x_{\text{min}} \) at \( x_{\text{C,peak}} \approx -6.4 \) \([30]\).
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