The specific heat of thin films near the $\lambda$-transition: a Monte Carlo study of an improved three-dimensional lattice model

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Abstract. We study the finite size scaling behaviour of the specific heat of thin films in the neighbourhood of the $\lambda$-transition. To this end we have simulated the improved two-component $\phi^4$ model on the simple cubic lattice. We employ free boundary conditions in the short direction to mimic the vanishing order parameter at the boundaries of a $^4\text{He}$ film. Most of our simulations are performed for the thicknesses $L_0 = 8, 16$ and $32$ of the film. It turns out that one has to take into account corrections $\propto L_0^{-1}$ to obtain a good collapse of the finite size scaling functions obtained from different $L_0$. Our results are compared with those obtained from experiments on thin films of $^4\text{He}$ near the $\lambda$-transition, from field theory and from 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 the neighbourhood of a second-order phase transition the behaviour of various quantities is governed by power laws. For example, the correlation length diverges as

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

(1)

where $t = (T - T_c)/T_c$ is the reduced temperature, $\xi_{0,\pm}$ are the amplitudes in the high and the low temperature phase, respectively, and $\nu$ is the critical exponent of the correlation length. $T_c$ is the critical temperature, where the phase transition occurs.\(^1\)

The specific heat behaves as

$$C \simeq A_{\pm} |t|^{-\alpha} + B,$$

(2)

where $A_+$ and $A_-$ are the amplitudes in the high and the low temperature phase, respectively, and $B$ is an analytic background, which has to be taken into account here, since

\(^1\) In the case of the $\lambda$-transition of $^4$He we shall denote the critical temperature by $T_\lambda$. 

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the critical exponent $\alpha$ of the specific heat is negative for the three-dimensional $XY$ universality class. A universality class is characterized by the dimension of the system, the range of the interaction and the symmetry of the order parameter. Critical phenomena can be understood in the framework of the renormalization group (RG). For reviews on critical phenomena and the renormalization group see e.g. [1]–[4]. The $XY$ universality class in three dimensions with short range interactions is of particular interest, since the $\lambda$-transition of $^4$He shares this universality class. Results for critical exponents and amplitude ratios such as $A_+/A_-$ obtained at the $\lambda$-transition are more precise than those from experiments on other systems.

It is an interesting question how the critical behaviour is modified by a confining geometry. If the system is finite in all directions, thermodynamic functions have to be analytic functions. That is, a singular behaviour like that of equations (1), and (2) is excluded. As a remnant of such singularities there remains a peak in the neighbourhood of the transition. With increasing linear extension the height of the peak increases and the temperature of the maximum approaches the critical temperature. This behaviour is described by the theory of finite size scaling (FSS). For reviews see [5,6].

In the present work we study thin films. Thin films are finite in one direction and infinite in the other two directions. In this case 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 [7]–[9] is expected. In our recent work [10] we have focused on the study of this transition and the scaling of the transition temperature with the thickness of the film.

Here we investigate the behaviour of the specific heat of thin films in the neighbourhood of the $\lambda$-transition. The specific heat has been studied in a number of experiments on thin films of fluid $^4$He and $^3$He–$^4$He mixtures near the $\lambda$-transition. For recent reviews see [11,12].

The physics of thin films is governed by the ratio $L_0/\xi$, where $\xi$ is a correlation length of the bulk system and $L_0$ the thickness of the thin film. For $L_0 \gg \xi$ the behaviour of the film is essentially given by the thermodynamic limit of the three-dimensional system. In the critical region, when $\xi$ gets close to $L_0$ or even larger, the behaviour deviates from the three-dimensional one and is characterized by universal functions of $L_0/\xi$. These universal functions depend on the type of the boundary conditions that the surface of the system imposes on the order parameter.

In particular, the behaviour of the specific heat can be described by the universal scaling function

$$[C_{\text{bulk}}(t) - C(t, L_0)] A^{-1} |t|^\alpha \simeq g_{2,R}(L_0/\xi) \simeq g_{2,R}(t[L_0/\xi_0]^{1/\nu}),$$

where $C_{\text{bulk}}(t)$ is the specific heat of the three-dimensional thermodynamic limit and $C(t, L_0)$ the specific heat of a film of thickness $L_0$. As $A$ either $A_+$ or $A_-$ can be taken and analogously as $\xi_0$ either $\xi_{0,+}$ or $\xi_{0,-}$. In the last step of the equation we have used equation (1). Following RG theory, the analytic background $B$ is the same for the bulk and the thin film. Therefore it cancels in the difference that is considered here. Alternatively

2 Note that also other confining geometries like cubes or pores have been studied experimentally and theoretically, in particular by using Monte Carlo simulations of lattice models. For a discussion of these studies we refer the reader to the review [12].

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one might consider

$$[C_{\text{bulk}}(t_0) - C(t, L_0)]A^{-1}|t|^\alpha \simeq \tilde{g}_{1,R}(L_0/\xi) \simeq g_{1,R}(t[L_0/\xi_0]^{1/\nu}),$$

where $t_0$ is chosen such that $\xi(t_0) = L_0$ in the high temperature phase. Multiplying equations (3) and (4) by $(|t|L_0/\xi_0)^{1/\nu})^{-\alpha}$ one arrives at

$$[C_{\text{bulk}}(t) - C(t, L_0)]A^{-1}\xi_0^{\alpha/\nu}L_0^{-\alpha/\nu} \simeq \tilde{f}_{2,R}(L_0/\xi) \simeq f_{2,R}(t[L_0/\xi_0]^{1/\nu})$$

and

$$[C_{\text{bulk}}(t_0) - C(t, L_0)]A^{-1}\xi_0^{\alpha/\nu}L_0^{-\alpha/\nu} \simeq \tilde{f}_{1,R}(L_0/\xi) \simeq f_{1,R}(t[L_0/\xi_0]^{1/\nu})$$

respectively. Often in the literature the factors $A^{-1}$ and $A^{-1}\xi_0^{\alpha/\nu}$ are omitted and $tL_0^{1/\nu}$ is used as the argument of the scaling function. This poses no problem as long as films of different thicknesses of the same system are considered. However, comparing films of e.g. $^4$He at different pressures or $^3$He–$^4$He mixtures at different concentrations of $^3$He this fact has to be taken into account. The same holds for the comparison of such experimental results with those obtained from lattice models or field theory. In the following we shall use the notation $f_1 = A\xi_0^{-\alpha/\nu} f_{1,R}$ and $f_2 = A\xi_0^{-\alpha/\nu} f_{2,R}$.

These scaling functions have been determined by a number of experiments on $^4$He and mixtures of $^3$He and $^4$He. In the high temperature phase, the data follow nicely the prediction of finite size scaling as can be seen e.g. from figure 14 of [12]. In this figure, $[C_{\text{bulk}}(t) - C(t, L_0)]/|t|^\alpha$ is plotted as a function of $|t|L_0/\xi_0]^{1/\nu}$ for films of $^4$He at vapour pressure of thicknesses 483 Å up to 57 μm. The data for different thicknesses fall nicely on top of each other. In their figure 20 the authors of [12] have plotted data for the low temperature phase in an analogous way. Up to $|t|L_0^{1/\nu} \approx 5$ the data for different thicknesses fall nicely on top of each other. However for larger values of $|t|L_0^{1/\nu}$ the data start to scatter. This is most pronounced at $|t|L_0^{1/\nu} \approx 10$, where the function assumes a minimum. There is a factor of about 3.5 between the value for the thinnest and the value for the thickest film. From $|t|L_0^{1/\nu} \approx 20$ up to 100 there is a factor of about 2 between the thinnest and the thickest of the films. Note that in figure 20 of [12] $L_0$ is given in Å and $t = 1 - T/T_\lambda$.

In the case of superfluid helium the order parameter is a complex wavefunction. This wavefunction vanishes at the boundaries of the film. In order to mimic this in theoretical models, Dirichlet boundary conditions with vanishing field are employed.

Using such boundary conditions, the scaling function $f_2$ has been calculated by using the $\epsilon$-expansion to $O(\epsilon)$ [13,14]. The coefficients of $O(1)$ and $O(\epsilon)$ are numerically of similar size. Therefore one should not expect quantitatively accurate results for $f_2$ obtained this way. Both $f_1$ and $f_2$ have been computed by using perturbation theory in three dimensions fixed [15]–[17] in the one-loop approximation. In the high temperature phase and at the critical point of the bulk system, the experimental results are fairly well reproduced. However in the low temperature phase, in particular close to the KT transition, no accurate predictions can be obtained.

Also Monte Carlo simulations of the standard XY model on a simple cubic lattice have been performed to determine the specific heat of thin films. For a precise definition of the XY model see below. In [18] staggered boundary conditions have been used to obtain a vanishing order parameter at the boundaries. The authors of [20] have employed

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free (in their notation ‘open’) boundary conditions as we do in the present work. In both cases the authors have computed the finite size scaling function $f_1$. In [18, 19] the authors have simulated lattices of a thickness up to $L_0 = 24$ lattice units, while in [20] the thicknesses $L_0 = 12$, 14 and 16 have been studied. The results of [18, 19] and [20] for $f_1$ agree. There is also a reasonable match with experiments on helium films. In [21] thin films with periodic boundary conditions have been studied. As can be seen from figure 15 of [19], the finite size scaling function $f_1$ obtained for boundary conditions of this type is clearly different from that for staggered or free boundary conditions.

The purpose of the present paper is to compute the finite size scaling function $f_2$ for the first time by using Monte Carlo simulations of a lattice model. Furthermore we carefully study corrections to scaling, allowing us to quantify the error of our result for the finite size scaling function.

For finite systems we expect the leading correction to be $\propto L_0^{-\omega}$, irrespective of the type of the boundary conditions [5]. The numerical value of the correction exponent is $\omega = 0.785(20)$ for the $XY$ universality class in three dimensions [22]; similar results are obtained with field theoretic methods; see e.g. [4]. In order to avoid these corrections, we study an improved model. In improved models the amplitude of corrections $\propto L_0^{-\omega}$ vanishes or, in practice, it is so small that its effect can be ignored. The precise definition of the model that we have simulated is given below.

On top of the restricted geometry, free boundary conditions introduce new physical effects. For a discussion see e.g. reviews on surface critical phenomena [23, 24]. In fact, free boundary conditions lead to additional corrections to scaling. The leading one is $\propto L_0^{-1}$ [25]; it can be cast in the form $L_{0,\text{eff}} = L_0 + L_s$. In [10] we have obtained the accurate numerical estimate $L_s = 1.02(7)$ for the model that we simulate here.

This paper is organized as follows. In section 2 we define the lattice model that we have simulated and the observables that we have computed. In section 3 we discuss how corrections caused by the free boundary conditions affect the finite size scaling behaviour of the specific heat. Next we discuss the details of our simulations. On the basis of these simulations we compute the scaling functions $f_1$ and $f_2$. We compare our results with those from experiments on thin films of $^4$He, field theoretic methods and previous Monte Carlo simulations.

2. The model and the observables

2.1. The two-component $\phi^4$ model

We study the two-component $\phi^4$ model on a 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- and 2-directions we employ periodic boundary conditions and we use free boundary conditions in the 0-direction. This means that the sites with $x_0 = 1$ and $L_0$ have only five nearest neighbours. This type of boundary conditions could be interpreted as Dirichlet boundary conditions with 0 as the value of the field at $x_0 = 0$ and $L_0 + 1$. Note that, viewed this way, the thickness of the film is $L_0 + 1$ rather than $L_0$. This provides a natural

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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 [26] in the context of the surface susceptibility of Ising films.

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explanation of the result \( L_s = 1.02(7) \) obtained in [10] 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

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

(7)

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

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

(8)

Note that following the conventions of our previous work, e.g. [28], 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; 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 \( \lambda^* = 2.10(6) \) [27], \( \lambda^* = 2.07(5) \) [28] and most recently \( \lambda^* = 2.15(5) \) [22]. The inverse of the critical temperature \( \beta_c \) has been determined accurately for several values of \( \lambda \) using finite size scaling (FSS) [22]. 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 [10, 22, 29, 30]. At \( \lambda = 2.1 \) one gets \( \beta_c = 0.5091503(6) \) [22]. Since \( \lambda = 2.1 \) is not exactly equal to \( \lambda^* \), there are still corrections that are \( \propto L_0^{-\alpha} \), although with a small amplitude. In fact, following [22], it should be by at least a factor 20 smaller than for the standard XY model.

2.2. The energy and the specific heat

First we should note that in equation (7) \( \beta \) does not multiply the second term. Therefore, strictly speaking, \( \beta \) is not the inverse temperature. However, 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 smooth and not tangent to the transition line. Here, for computational convenience, we vary \( \beta \) at fixed \( \lambda \). Correspondingly we define the energy density as the derivative of the reduced free energy density with respect to \( \beta \). Furthermore we multiply by \(-1\) to get positive numbers:

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

(9)

It follows that

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

(10)

\(^4\) Therefore, following [3] we actually should call it the reduced Hamiltonian.

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We then define the specific heat as the derivative of the energy density with respect to $\beta$: \[ C = \frac{\partial E}{\partial \beta}. \] (11)

It is easy to show that \[ C = \frac{1}{L_0 L_1 L_2} \left( \left\langle \left[ \sum_{(x,y)} \vec{\phi}_x \cdot \vec{\phi}_y \right]^2 \right\rangle - \left\langle \sum_{(x,y)} \vec{\phi}_x \cdot \vec{\phi}_y \right\rangle^2 \right). \] (12)

2.3. The correlation length

The second-moment correlation length $\xi_{2nd}$ and the transverse correlation length $\xi_T$ of the bulk system are used to set the scale in the high and the low temperature phase, respectively. Here we shall use the results given in [30]. For completeness we recall the definitions of the two correlation lengths.

The second-moment correlation length in the $k$-direction is defined by \[ \xi_{2nd,k} = \sqrt{\frac{\chi/F_k - 1}{4 \sin(\pi/L_1)^2}}, \] (13)

where \[ \chi = \frac{1}{L_0 L_1 L_2} \left\langle \tilde{M}^2 \right\rangle \] (14)

is the magnetic susceptibility and \[ F_k = \frac{1}{L_0 L_1 L_2} \left\langle \left| \sum_x \exp \left( \frac{2\pi x_k}{L_k} \right) \hat{\phi}_x \right|^2 \right\rangle \] (15)

is the Fourier transform of the correlation function at the lowest non-zero momentum in the $k$-direction. Note that in the high temperature phase there is 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 [28],

\[ \lim_{t \to 0} \frac{\xi_{exp}}{\xi_{2nd}} = 1.000 \, 004(3) \quad (t > 0) \] (16)

for the thermodynamic limit of the three-dimensional system. In [10] we find for $\lambda = 2.1$, by fitting the data for the second-moment correlation length for $\beta \geq 0.49$,

\[ \xi_{2nd} = 0.263 \, 62(8) t^{-0.6717} \times [1 + 0.039(8) t^{0.527} - 0.72(4) t], \] (17)

where $t = 0.509 \, 1503 - \beta$.

The helicity modulus $\Upsilon$ gives the reaction of the system under a torsion. To define the helicity modulus we consider a system where rotated boundary conditions are introduced in one direction (e.g. the 1-direction): for $x_1 = L_1$ and $y_1 = 1$ the term $\vec{\phi}_x \vec{\phi}_y$ in the Hamiltonian is replaced by \[ \vec{\phi}_x \cdot R_{\alpha} \vec{\phi}_y = \phi_x^{(1)} (\cos(\alpha) \phi_y^{(1)} + \sin(\alpha) \phi_y^{(2)}) + \phi_x^{(2)} (-\sin(\alpha) \phi_y^{(1)} + \cos(\alpha) \phi_y^{(2)}). \] (18)

Throughout, in the context of the $\phi^4$ model we use the convention $t = \beta - \beta$. 

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The helicity modulus is then given by
\[
\Upsilon = -\frac{L_1}{L_0 L_2} \frac{\partial^2 \log Z(\alpha)}{\partial \alpha^2} \bigg|_{\alpha=0}.
\]  
(19)

Note that we have skipped a factor of \(T\) compared with the standard definition [31]. Defined this way, the helicity modulus has the dimension of an inverse length. In the literature \(\xi_\perp = 1/\Upsilon\) is referred to as the transverse correlation length. Fitting the data for the helicity modulus at \(\lambda = 2.1\), given in table 2 of [30], up to \(\beta = 0.55\), we get
\[
\Upsilon = 1.5584(10)(-t)^{0.6717} \times (1 + 0.06(2)t),
\]  
(20)
with \(t = 0.5091503 - \beta\).

3. The finite size scaling behaviour of the specific heat

In this section we discuss the finite size scaling behaviour of the specific heat of thin films. The reduced free energy density of the bulk system is given by
\[
f_{\text{bulk}}(t) = \tilde{\alpha} t^{-\alpha} (1 + c_1 t^\theta + c_2 t^{2\theta} + d_1 t^{\theta'} + e_1 t + \cdots) + b(t),
\]  
(21)
where \(b(t)\) is the analytic background, \(e_1 t\) is an analytic correction and \(c_1 t^\theta\), \(c_2 t^{2\theta}\) and \(d_1 t^{\theta'}\) are non-analytic corrections. In order to simplify the notation, we have omitted subscripts \(\pm\) that indicate the phase. Numerical values of the corrections exponents are \(\theta = \nu \omega \approx 0.527\) [22] and \(\theta' \approx 1.2\) [32]. Note that the correction amplitudes \(c_1, c_2, \ldots\) are small for the \(\phi^4\) model at \(\lambda = 2.1\), while \(d_1\) and \(e_1\) should assume generic values. In the following discussion we shall, for simplicity, ignore these corrections to scaling. Inserting \(\xi(t) = \xi_0 t^{-\nu}\) into equation (21) we arrive at
\[
f_{\text{bulk}}(t) = [\tilde{\alpha} \xi_0^d] \xi(t)^{-d} + b(t),
\]  
(22)
where we have used the hyperscaling relation \(2 - \alpha = d \nu\), where \(d\) is the dimension of the system. Note that \(\tilde{\alpha} \xi_0^d\) is universal.

The reduced free energy density of a thin film with periodic boundary conditions with the thickness \(L_0\) is given by [5]
\[
f_P(t, L_0) = L_0^{-d} q_P(t[L_0/\xi_0]^{1/\nu}) + b(t),
\]  
(23)
where \(d\) is the dimension of the system and \(b(t)\) in equation (23) is the same function as in equation (21). Also \(q_P(x)\) is an analytic function at \(x = 0\). There might be a singularity at some \(x \neq 0\) related with the effectively two-dimensional transition. In order to eliminate the analytic background one considers the difference
\[
f_{\text{bulk}}(t) - f_P(t, L_0) = L_0^{-d} [\tilde{\alpha} \xi_0^d] (L_0/\xi(t))^{-d} q_P(t[L_0/\xi_0]^{1/\nu})
\]  
\[
= L_0^{-d} p_P(t[L_0/\xi_0]^{1/\nu}).
\]  
(24)

The specific heat is defined as minus the second derivative of \(f\) with respect to an analytic function \(h(t)\). Using our definitions, it is minus the second derivative with respect to \(t\) itself. Applying this to equation (21) we arrive at \(A = -h'(0)^{-2}(1-\alpha)(2-\alpha)\tilde{\alpha}\) for the amplitude of the specific heat. Taking minus the second derivative of equation (24) with
In the case of free boundary conditions, which are studied in the present work, boundary effects have to be taken into account. In [10] we have numerically shown that leading corrections can be accounted for by replacing $L_0$ by $L_{0,\text{eff}} = L_0 + L_s$, where we have obtained the estimate $L_s = 1.02(7)$. Hence

$$\frac{L_0}{L_{0,\text{eff}}^2} f_F(t, L_0) = L_{0,\text{eff}}^{-d} q_F(t[L_{0,\text{eff}}/\xi_0]^{1/\nu}) + b(t) + c(t)L_{0,\text{eff}}^{-1}. \quad (26)$$

The additional term $c(t)L_{0,\text{eff}}^{-1}$ gives a correction of the analytic background caused by the free boundary conditions. Written this way it allows that the correction to the background is given by an effective thickness that is different from $L_{0,\text{eff}}$. The prefactor $(L_0/L_{0,\text{eff}})$ in front of $f_F(t, L_0)$ corrects the volume that is used to compute the reduced free energy density.

Taking the same steps as in the case of periodic boundary conditions we arrive at

$$C_{\text{bulk}}(t) - C_F(t, L_0) = -h(0)^{-2}\left[L_0^{-d}[L_0/\xi_0]^{3/\nu}p_F'(t[L_0/\xi_0]^{1/\nu}) \right. \quad (25)$$

In the high temperature phase,

$$C_{\text{bulk}}(t) - C_F(t, L_0) = -h(0)^{-2}\tilde{a}[L_0/\xi_0]^{\alpha/\nu}[\tilde{a}^{\nu}][\tilde{a}^{\nu}]^{-1}p_F'(t[L_0/\xi_0]^{1/\nu}) \quad (25)$$

where $\xi(t_0) = L_0$ or better $\xi(t_0) = L_{0,\text{eff}}$ for $t_0$ in the high temperature phase.

Here we study the neighbourhood of the critical point. Therefore we shall use the approximation $w(t) \approx w(0)$. To simplify the notation we shall write $w$ instead of $w(0)$ in the following.

$$\left[C_{\text{bulk}}(t) - C_F(t, L_0)\right]_{L_0^{-\alpha/\nu}} = A\xi_0^{-\alpha/\nu} f_2(t[L_0/\xi_0]^{1/\nu}) - w(t) L_{0,\text{eff}}^{-1-\alpha/\nu}. \quad (27)$$

$$\left[C_{\text{bulk}}(t) - C_F(t, L_0)\right]_{L_0^{-\alpha/\nu}} = A\xi_0^{-\alpha/\nu} f_2(t[L_0/\xi_0]^{1/\nu}) - w(t) L_{0,\text{eff}}^{-1-\alpha/\nu}, \quad (28)$$

Note that for large $|t|[L_{0,\text{eff}}/\xi_0]^{1/\nu}$ the difference $|C_{\text{bulk}}(t_0) - (L_0/L_{0,\text{eff}})C_F(t, L)|$ becomes small compared with $C_{\text{bulk}}(t_0)$ or $C_F(t, L)$. On the other hand, corrections due to the boundary are virtually independent of $|t|[L_{0,\text{eff}}/\xi_0]^{1/\nu}$. Therefore corrections due to the boundary might lead to large relative errors for large values of $|t|[L_{0,\text{eff}}/\xi_0]^{1/\nu}$.

4. Numerical results

4.1. The thermodynamic limit of the three-dimensional system

In this subsection we shall consider systems with periodic boundary conditions in all three directions and the linear size $L_0 = L_1 = L_2 = L$. In the high temperature phase, corrections to the thermodynamic limit decay exponentially with increasing lattice size. In practice it turns out that for $L \gtrsim 10\xi_{2\text{nd}}$, these corrections are much smaller than the statistical error that we reach here. Since a Goldstone mode is present in the low temperature phase of the system [33, 34], corrections to the thermodynamic limit decay only with some power of the linear lattice size. In particular for the energy density and

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the specific heat, we expect that, to leading order, the correction decays \(\propto L^{-3}\). Therefore rather large lattices are needed to get a good approximation of the thermodynamic limit.

One should note that the estimator (10) of the energy density is self-averaging, while the one (12) for the specific heat is not. Since the lattices have to be rather large to avoid sizable finite size effects, it turns out that the specific heat can be most efficiently determined by fitting the energy density in some range of \(\beta\).

To this end, we have computed the energy density for a large number of \(\beta\)-values. As the starting point we have taken the data given in tables 2 and 5 of [30]. These were supplemented by a rather large number of new simulations to obtain a dense grid of \(\beta\)-values. In particular, we have simulated the 96\(^3\) lattice in the range 0.521 \(\leq \beta \leq 0.58\) in steps of \(\Delta \beta = 0.0005\), for 0.5025 \(\leq \beta \leq 0.5035\) in steps of \(\Delta \beta = 0.0001\) and for \(\beta = 0.491\), 0.492, 0.494, 0.496, 0.497, 0.498, 0.499, 0.501, 0.502, 0.503 and 0.504. We simulated the 128\(^3\) lattice at \(\beta = 0.516\), 0.517, 0.518, 0.519 and 0.5205, the 192\(^3\) lattice at \(\beta = 0.514\), 0.5145, 0.5155, 0.5165, 0.5175, 0.5185 and 0.5195 and finally the 288\(^3\) lattice at \(\beta = 0.5115\), 0.5125, 0.5135, and 0.5145.

In the case of \(L = 96\) we typically performed \(10^5\) measurements and \(5 \times 10^4\) for the larger lattice sizes. For each of these measurements a Metropolis sweep, several overrelaxation sweeps and single-cluster [35] updates were performed. For a discussion of the Monte Carlo algorithm see [30]. In total, these simulations took a little less than one year of CPU time on one core of a 2218 Opteron processor (2.60 GHz).

In [30] the results for the thermodynamic limit in the low temperature phase were obtained by fitting the data for several lattice sizes with the ansatz \(E(L) = E(\infty) + cL^{-3}\). In the case of the simulations that we have added here, we have checked that the \(cL^{-3}\) corrections are sufficiently small to be ignored.

In the neighbourhood of the transition, we have fitted the energy density with the ansatz
\[
E(\beta) = E_{\text{ns}} + C_{\text{ns}}(\beta - \beta_c) + a_\pm|\beta - \beta_c|^{1-\alpha} + d_{\text{ns}}(\beta - \beta_c)^2 + b_\pm|\beta - \beta_c|^{2-\alpha},
\]
(29)
where \(E_{\text{ns}}, C_{\text{ns}}, \beta_c = 0.5091503(6)\) and \(\alpha = -0.0151(3)\) [22] are input and \(a_\pm, d_{\text{ns}}\) and \(b_\pm\) are the five free parameters of the fit.

From the finite size scaling behaviour of \(L^3\) systems with periodic boundary conditions in all directions at the critical point we find [29]
\[
E_{\text{ns}} = 0.913213(5) + 20 \times (\beta_c - 0.5091503) + 5 \times 10^{-7} \times (1/\alpha + 1/0.0151)
\]
(30)
for the non-singular part of the energy density and
\[
C_{\text{ns}} = 157.9(5) + 147000 \times (\beta_c - 0.5091503) - 2.1 \times (1/\alpha + 1/0.0151)
\]
(31)
for the non-singular part of the specific heat at \(\lambda = 2.1\).

We did not include a term with the exponent \(1 - \alpha + \nu \theta' \approx 2\) in the ansatz (29). We expect that it is effectively taken into account by the last two terms in (29). Note that the main purpose of fitting the energy density with ansatz (29) is to interpolate our data in a large range of \(\beta\)-values.

After some preliminary studies, we decided to fit the energy density in the range 0.49 \(\leq \beta \leq 0.529\) using (29). In total we have 98 data points in this interval and we get \(\chi^2/\text{d.o.f.} = 1.08\) for our fit. The results for the fit parameters are \(a_+ = 160.688(2), a_- = -151.459(2), d_{\text{ns}} = -302.6(9.8), b_+ = 302.4(10.3)\) and \(b_- = 293.4(10.3)\).
The specific heat of thin films near the \( \lambda \)-transition

Figure 1. We plot our result for the specific heat obtained from the fit of the energy density using ansatz (29). Note that at \( \beta_c = 0.509 \pm 0.1503(6) \) the specific heat assumes the value \( C_{ns} = 157.9(5) \), equation (31). In addition to the result obtained by using the central values of the input parameters, we have also plotted those where we have replaced the central value by the central value plus the error. For example, \( C_{ns} = 157.9 \) is replaced by \( C_{ns} = 158.4 \). At the resolution of the plot, all these curves fall on top of each other. For a more detailed discussion see the text.

First we have computed the universal combination

\[
R_\alpha = (1 - A_+/A_-)/\alpha
\]

from the result of the fit. Note that \( A_+/A_- = -a_+/a_- \). Using the central values for the input parameters we obtain \( R_\alpha = 4.035(16) \), where we have taken into account the covariance of \( a_+ \) and \( a_- \). Furthermore we have checked the dependence of our result on the input parameters. In fact, the dependence on the value of \( \alpha \) is quite small. Taking the preferred value of the experiment on the space shuttle [36] \( \alpha = -0.0127 \) we get \( R_\alpha = 4.022(16) \). We have also checked the effect of the error of the other input parameters. It turns out that the uncertainty of \( C_{ns} \) has the largest effect on \( R_\alpha \): replacing \( C_{ns} = 157.9 \) by \( C_{ns} = 158.4 \) we get \( R_\alpha = 4.025(16) \). As our final result we quote

\[
R_\alpha = 4.035(16)[20],
\]

where in () we give the statistical error and in [] the sum of all errors due to the uncertainty of the input parameters of the fit. Note that the present result is compatible with the final result \( R_\alpha = 4.01(5) \) given in [29].

In figure 1 we have plotted the specific heat obtained from the fit of the energy density using ansatz (29). Computing the statistical error, correlations among the fit parameters are properly taken into account. In this plot, errors cannot be resolved. In order to make the errors visible we have plotted in figure 2 the statistical error and the difference between

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Figure 2. Various sources of the error of the specific heat as obtained from fits of the energy density using ansatz (29). We plot the statistical error (stat) and the difference of the result using the central values of the input parameters and results where we have replaced the central value of one of the input parameters by the central value plus the error. In particular, we have replaced \( C_{ns} = 157.9 \) by \( C_{ns} = 158.4 \) (Cns), \( E_{ns} = 0.913213 \) by \( E_{ns} = 0.913218 \) (ens), \( \beta_c = 0.5091503 \) by \( \beta_c = 0.5091509 \) (bc) and \( \alpha = -0.0151 \) by \( \alpha = -0.0148 \) (alpha). For a discussion see the text.

As one might expect, the differences diverge in the neighbourhood of the critical point. In the low temperature phase the largest uncertainty is due to the error of \( C_{ns} \). In particular, going to the upper boundary \( \beta = 0.529 \) of our fit interval, the uncertainty induced by the error of \( C_{ns} \) rapidly increases. Therefore we decided to use the values for the specific heat obtained from the fit (29) only up to \( \beta = 0.525 \). For larger values of \( \beta \) we follow an alternative approach as discussed below. In the case of the high temperature phase we shall use the results obtained from the fit (29) down to \( \beta = 0.49 \).

In order to complete the computation of the specific heat, we have fitted our data for the energy density with the ansatz

\[
E(\beta) = \sum_{i=0}^{n} a_i (\beta - \beta_0)^i, \tag{34}
\]

where \( a_i \) is identified with the specific heat at \( \beta_0 \). We have included all values of \( \beta \) within the interval \([\beta_0 - \Delta, \beta_0 + \Delta]\) into the fit. We have tested various values of \( n \). Our final results are taken from fits with \( n = 4 \). In the range \( 0.525 < \beta_0 < 0.529 \) we have used \( \Delta = 0.008 \). For \( 0.529 < \beta_0 < 0.537 \) we have used \( \Delta = 0.011 \) and for \( 0.537 \leq \beta_0 \leq 0.58 \) we have used \( \Delta = 0.016 \). In all cases \( \chi^2/\text{d.o.f.} \) is close to 1. To give an impression of the accuracy that is reached, we quote \( C = 12.690(3) \) at \( \beta = 0.525 \) and \( C = 11.899(2) \) at \( \beta = 0.53 \).

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For comparison with the results obtained from the fit with ansatz (29) we have also performed fits with ansatz (34) in the range $0.522 \leq \beta_0 \leq 0.525$ using $\Delta = 0.005$. The numerical results for the specific heat obtained from the two different approaches are compatible within error bars.

4.2. Adjusting the scale of the axes

As we have mentioned already in the introduction, often in the literature the factor $A^{-\alpha/\nu}$ is ignored when computing the finite size scaling functions $f_1$ and $f_2$. Therefore, in order to compare the results of different systems, we have to compute

$$r_{1,2} = \frac{[A\xi_0^{-\alpha/\nu}]_{\text{system 1}}}{[A\xi_0^{-\alpha/\nu}]_{\text{system 2}}}.$$  \hspace{1cm} (35)

In order to fix the ratio between our definition for the specific heat of the $\phi^4$ model at $\lambda = 2.1$ and that of experiments on $^4$He at vapour pressure, we take the ratio of our result for $A_-$ obtained in the previous subsection and that of [36] for the three-dimensional thermodynamic limit of $^4$He at vapour pressure. From table II of [36] we read off $\alpha A_- = 5.6950$. Using an alternative fit ansatz the authors get $\alpha A_- = 5.6950$. We regard this difference as an estimate of the possible error of $\alpha A_-$. From the same fits, the authors obtain $\alpha = -0.01264$ and $-0.01321$, respectively. In order to match with these experimental numbers, we have taken $\alpha A_- = 2.285$ obtained from fitting the energy density with ansatz (29), using $\alpha = -0.0127$ as input. Instead, using $\alpha = -0.0151$ we arrive at $\alpha A_- = 2.322$. That is, the value of $\alpha A_-$ is quite insensitive on the value of $\alpha$ that is assumed.

Furthermore, we need the amplitude of the correlation length for $^4$He at vapour pressure in the high and the low temperature phase. For the transverse correlation length in the low temperature phase one finds ([37] and references therein)

$$\xi_T \approx 3.42 \text{ Å} t^{-\nu},$$  \hspace{1cm} (36)

where $t = 1 - T/T_\lambda$. Alternatively we can compute the amplitudes of the correlation lengths from $A_\pm$ using the results for the universal amplitude ratios

$$R_T^+ = \xi_{0,2nd}(\alpha A_+)^{1/3} = 0.3562(10),$$  \hspace{1cm} (37)

$$R_T^- = \xi_{0,T}(\alpha A_-)^{1/3} = 0.850(5)$$  \hspace{1cm} (38)

and

$$R_T = \frac{\xi_{0,2nd}}{\xi_{0,T}} = 0.411(2)$$  \hspace{1cm} (39)

given in [30]. To this end, we first have to convert the results for the specific heat of the experiment from J mol$^{-1}$ K$^{-1}$ into Å$^{-3}$. To this end we need the density $\rho_\lambda = 146.1087$ kg m$^{-3}$ [38] of $^4$He at the $\lambda$-transition and the Boltzmann constant $k_b = 1.38065 \ldots \times 10^{-23}$ J K$^{-1}$. We arrive at

$$\xi_{0,T} = 3.45(3) \text{ Å},$$  \hspace{1cm} (40)

Note that our definition of $A_\pm$ and that used in [36] differ by a factor of $\alpha$. 

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where we have taken into account the errors of $R^{-}\xi$ and of the experimental estimate of $\alpha A_\perp$. In the case of the high temperature phase we get
\[ \xi_{0,2nd} = 1.422(5) \text{ Å}, \]
where we have used
\[ \alpha A_+ = 1.05251 \times 5.6537 = 5.9506 \]
taken from table II of [36] as input and the error is estimated by using
\[ \alpha A_+ = 1.05490 \times 5.6950 = 6.0077 \]
retrieved from an alternative ansatz [36].

Now we are ready to compute the ratio
\[ \left( \frac{\xi_{0,4He}}{\xi_{0,\phi^4}} \right)^{-\alpha/\nu}, \]
where we can either use $\xi_{2nd}$ or $\xi_T$. We get 1.0386 using $\alpha = -0.0151$ and 1.0324 using $\alpha = -0.0127$.

Hence we arrive at
\[ r_{4He,\phi^4} = 2.57, \]
with a relative uncertainty of about 2%. Let us note that this number is only valid for $^4$He at vapour pressure and the $\phi^4$ model at $\lambda = 2.1$ and the particular definitions of the specific heat that have been used.

### 4.3. Finite size scaling at $\beta_{c,3D}$

First we performed simulations at the inverse transition temperature $\beta_{c,3D} = 0.5091503(6)$ [22] of the three-dimensional system. Here the correlation length of the thin film is relatively small; we find $\xi_{2nd,\text{film}}/L_{0,\text{eff}} \approx 0.416$. Hence already rather small ratios of $L_1/L_0$ are sufficient to approximate well the two-dimensional thermodynamic limit and therefore large values of $L_0$ can be reached. Furthermore, by construction $L_0/\xi_{3D} = 0$. Therefore this is an ideal location at which to accurately study the finite size scaling behaviour and in particular the corrections caused by free boundary conditions.

At the critical point of the three-dimensional system equation (27) reduces to
\[ \frac{L_0}{L_{0,\text{eff}}} C(t, L_0) = C_{\text{ns}} + c L_0^{\alpha/\nu} + w L_{0,\text{eff}}^{-1}, \]
where $C_{\text{ns}} = C_{\text{bulk}}(0) = 157.9(5)$ [29] and $c = -f_2(0)$.

All numbers for the specific heat discussed in this section are determined by using equation (12). As a first step, we have simulated the thickness $L_0 = 8$ for $L_1 = L_2 = 16, 24, 32, 48$ and 64. We conclude from these simulations that, at the level of our statistical error, the two-dimensional thermodynamic limit of the specific heat is reached for $L_1 = L_2 = 48$. On the basis of this result we performed simulations for $L_0 = 12, 16, 24, 32, 48$ and 64 with $L_1 = L_2 = 6L_0$ throughout. In all cases, we performed $10^6$ measurements, where for each measurement we performed one Metropolis sweep, two overrelaxation sweeps and wall cluster [39] and single-cluster updates. The number of
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Table 1. Results for the specific heat $C$ obtained by using equation (12) at
$\beta = 0.5091503$, which is the estimate of [22] for $\beta_{c,3D}$, for lattices of the size $L_1 = L_2 = 6L_0$.

| $L_0$ | $C$     |
|-------|---------|
| 8     | 5.060(9)|
| 12    | 6.145(13)|
| 16    | 6.923(14)|
| 24    | 8.062(17)|
| 32    | 8.924(19)|
| 48    | 10.141(24)|
| 64    | 11.000(29)|

Table 2. Fitting the data for the specific heat given in table 1 using ansatz (46).

| $L_{0,\text{min}}$ | $c$            | $w$            | $\chi^2$/d.o.f. |
|---------------------|-----------------|-----------------|-----------------|
| 8                   | $-161.569(14)$  | 3.32(16)        | 1.01            |
| 12                  | $-161.597(20)$  | 3.90(33)        | 0.21            |
| 16                  | $-161.595(25)$  | 3.85(53)        | 0.28            |

single-cluster updates was chosen such that the average size of a cluster times the number of clusters is a bit less than the number of lattice sites. In total these simulations took about five months of CPU time on one core of a 2218 Opteron processor (2.60 GHz). The results for the specific heat, as defined by equation (12), are summarized in table 1.

We have fitted these data with ansatz (46), where we have fixed $C_{ns} = 157.9$, $\beta_c = 0.5091503$, $\alpha = -0.0151$ and $L_s = 1.02$. The results of these fits are summarized in table 2. Already for $L_{0,\text{min}} = 12$ the $\chi^2$/d.o.f. is smaller than 1. Going to larger $L_{0,\text{min}}$ the statistical error of $w$ rapidly increases. Therefore we take the result obtained for $L_{0,\text{min}} = 12$ as our final result. On the basis of our data, it is impossible to give an estimate of systematic errors due to subleading corrections.

In order to check the dependence on the input parameters, we have repeated the fits for $L_{0,\text{min}} = 12$ using values of the input parameters that are shifted by the error of the input parameters: e.g. in one of these fits $L_s = 0.95$, while the other input parameters remain unchanged. In the case of $\alpha$ and $\beta_c$, we have taken into account the effect of the shift on $C_{ns}$ and $E_{ns}$ as given by equations (30), and (31). It turns out that shifting $L_s$ has the largest effect on $w$. Using $L_s = 0.95$ we get $w = 4.40(32)$. Taking the shifted value $C_{ns} = 158.4$ for the analytic background we get $w = 4.17(33)$. Shifting the other input parameters has less impact on the value of $w$.

Our result for $c = -f_2(0)$ can be compared with experiments and results obtained by field theoretic methods. On page 1028 in section V.A. of [12] the authors analyse the scaling behaviour of the specific heat of thin films at the $\lambda$-transition of the three-dimensional system. Fixing $\alpha = -0.01264$ they arrive at

$$C(0, L_0) = [453.8 \pm 4.3] - [474.0 \pm 4.9]L_0^{\alpha/\nu},$$

where $C$ is measured in units of J mol$^{-1}$ K$^{-1}$ and $L_0$ in Å.
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Analysing our data for the specific heat at $\beta_{c,3D}$, assuming $\alpha = -0.01264$, we arrive at $c \approx -190$. Multiplying with $r_{\text{He},\phi^4} = 2.57$ we arrive at $-488$, in quite good agreement with the experimental result $-[474.0 \pm 4.9]$, in particular when taking into account the error of $r_{\text{He},\phi^4}$.

We can also write our result in terms of the universal ratio

$$-f_{2,R}(0) = \frac{c}{A_+ \xi_{0,2nd}^{\alpha/\nu}} = 1.0208(2) - 1.33 \times (\alpha + 0.0151),$$

where the error quoted in ( ) is dominated by the statistical error of the specific heat of the thin films and the uncertainty of $L_x$. The dependence on the value of $\alpha$ that is used in the analysis is rather weak. The authors of [13] have computed $-f_{2,R}(0)$ (in their notation $\omega_{\text{OO}}$) using $\epsilon$-expansion to $O(\epsilon)$. Their result is given in their eq. (8.17). To leading order $\omega_{\text{OO}} = 1$, which is in quite good agreement with both our numerical result and with the experiment. Dohm and Sutter [17] have pointed out that the extrapolation to $\epsilon = 1$ is affected by considerable ambiguities. In fact, setting $\epsilon = 1$ the authors of [13] find $\omega_{\text{OO}} \approx 0.75$ (table II of [13]), which is clearly ruled out by our result as well as by experiment.

4.4. Finite size scaling at $\beta_{\text{KT}}(L_0)$

The KT phase transition occurs, up to scaling corrections, at a given value of the scaling variable $tL_0^{1/\nu}$ or equivalently $L_0/\xi_T$. In [10] we find $[L_0/\xi_T]^* = 1.595(7)$. Following the KT theory [7]–[9] the free energy is infinitely often differentiable with respect to the temperature at the KT transition. Therefore no particular problem for the numerical analysis is expected. At the KT transition equation (27) reduces to

$$C_{\text{bulk}}(\beta_{\text{KT}}(L_0)) - \frac{L_0}{L_{0,\text{eff}}} C(\beta_{\text{KT}}(L_0), L_0) = c_{\text{KT}} L_{0,\text{eff}}^{\alpha/\nu} - w L_0^{-1},$$

where $c_{\text{KT}}$ is $f_2$ at $[L_0/\xi_T]^* = 1.595(7)$.

We have obtained accurate data for several values of $L_0$ in relation with [10]. In table 3 we have summarized the results for the specific heat obtained by using equation (12) at the KT transition. The results that are quoted were obtained for $L_1 = L_2 = 32 L_0$ lattices. In the case of $L_0 = 24$ and 32, these are the largest available. For $L_0 < 24$ we have checked that the results obtained from $L_1 = L_2 = 32 L_0$ are consistent within the statistical error with those obtained from larger values of $L_1 = L_2$. In addition, we give numerical estimates for the specific heat of the three-dimensional bulk system as discussed in section 4.1.

We have fitted these data with ansatz (49). Our results, using the central values of the input parameters, are summarized in table 4. The value of $w$ is increasing with increasing minimal thickness $L_{0,\text{min}}$ that is included into the fit. The result obtained for $L_{0,\text{min}} = 16$ is compatible within the statistical error with that obtained in the preceding subsection for $\beta_{c,3D}$.

Next, we have checked how the results for $c_{\text{KT}}$ and $w$ depend on the values of the input for $L_s$ and $\alpha$. To this end we have repeated fits for $L_{0,\text{min}} = 16$ using shifted values for these input parameters. Using $\alpha = -0.0151$ and $L_s = 0.95$ as input we get $c_{\text{KT}} = 0.634(42)$ and $w = 3.61(65)$. Changing the value of the exponent of the specific heat to $\alpha = -0.0148$ and keeping $L_s = 1.02$ we get $c_{\text{KT}} = 0.649(42)$ and $w = 3.03(66)$. Finally we have set

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Table 3. Results for the specific heat at the KT transition of thin films. In the first column we give the thickness \( L_0 \) of the film; in the second column, we give the result for \( \beta_{KT}(L_0) \) obtained in [10]. In the third column we give the estimate of the specific heat \( C_{\text{bulk}} \) of the three-dimensional bulk system at this temperature and finally, in the fourth column the specific heat of the thin film at the KT transition. Throughout we have taken the result for \( L_1 = L_2 = 32L_0 \).

For a detailed discussion see the text.

| \( L_0 \) | \( \beta_{KT} \) | \( C_{\text{bulk}} \) | \( C_{\text{film}} \) |
|--------|---------|---------|---------|
| 6      | 0.56825(1) | 8.586(1) | 9.710(15) |
| 8      | 0.549278(5) | 9.870(1) | 10.793(17) |
| 12     | 0.532082(3) | 11.617(2) | 12.179(20) |
| 16     | 0.524450(2) | 12.791(7) | 13.176(23) |
| 24     | 0.517730(2) | 14.342(5) | 14.454(22) |
| 32     | 0.514810(1) | 15.379(6) | 15.311(33) |

Table 4. Fits of the specific heat \( C \) at the KT transition with ansatz (49). Data with \( L_{0,\text{min}} \leq L_0 \leq 32 \) are included into the fit. We have fixed \( \alpha = -0.0151 \) and \( L_s = 1.02 \).

| \( L_{0,\text{min}} \) | \( c_{KT} \) | \( w \) | \( \chi^2/\text{d.o.f.} \) |
|---------------------|---------|------|-----------------|
| 8                   | 0.587(21) | 2.07(19) | 2.98 |
| 12                  | 0.638(27) | 2.81(31) | 1.00 |
| 16                  | 0.650(42) | 3.04(66) | 1.42 |

\( \alpha = -0.0127 \) obtained from the space shuttle experiment [36]. Keeping \( L_s = 1.02 \) we get \( c_{KT} = 0.641(41) \) and \( w = 2.99(65) \).

As one might expect, \( w \) shows a strong dependence on the value of \( L_s \). On the other hand the dependence of \( w \) on \( \alpha \) is quite weak; even using the preferred value of [36] the results for \( c_{KT} \) and \( w \) change only little. As our final estimate we take \( c_{KT} = 0.65(4) \) and \( w = 3.5 \) in the following analysis of the specific heat over a large range of the scaling variable. The error of \( w \) should be about 1.

4.5. Specific heat for \( L_0 = 8, 16 \) and 32 for a large range of \( \beta \)

Finally we have computed the specific heat for \( L_0 = 8, 16 \) and 32 for a large range of \( \beta \) in the neighbourhood of \( \beta_{c,3D} \). For this purpose, it turns out to be more efficient to compute the specific heat by taking the derivative of the energy density (10) with respect to \( \beta \) numerically than by using equation (12).

Let us first discuss how we have computed the two-dimensional thermodynamic limit of the energy density of the thin films. In the high temperature phase of the thin film we expect the energy density to converge exponentially fast with increasing \( L = L_1 = L_2 \) toward the effectively two-dimensional thermodynamic limit. In order to see this asymptotic behaviour, lattices with \( L \gg \xi_{2\text{nd},\text{film}} \) are needed. From numerical results for the two-dimensional \( XY \) model we conclude that \( L \gtrsim 8\xi_{2\text{nd},\text{film}} \) is needed such that the deviation from the thermodynamic limit is far smaller than the statistical error that
we typically reach in our study. For \( L_0 = 8, 16 \) and 32 we have simulated lattices up to \( L = 2048, 1800 \) and 1024, respectively. Therefore we were able to satisfy the condition \( L \gtrsim 8\xi_{\text{2nd, thin}} \) up to \( \beta = 0.545, \beta = 0.522 \) and \( \beta = 0.5134 \), respectively. At these values of \( \beta \) we find \( \xi_{\text{2nd, thin}} = 242.5(2), 153.16(15) \) and 111.99(15) for films of the thickness \( L_0 = 8, 16 \) and 32, respectively.

For \( \beta > \beta_{\text{KT}} \) the asymptotic behaviour is given by the spin-wave approximation; i.e. by a free field theory. Therefore the thermodynamic limit is approached as \( E(L) = E(\infty) + O(L^{-2}) \). In this range of \( \beta \) we have taken \( E(\infty) = \frac{1}{c}[4E(2L) - E(L)] \) as our final result for the thermodynamic limit.

Unfortunately there is a quite large range of \( \beta \) where the extrapolation to the thermodynamic limit is less clear: \( \beta_{\text{max}} < \beta \leq \beta_{\text{KT}} \), where \( \beta_{\text{max}} \) is the largest value of \( \beta \) such that \( L_{\text{max}} \gtrsim 8\xi_{\text{2nd}} \) and \( L_{\text{max}} \) is the largest lattice size that we can simulate with our (finite) computer resources.

In the context of [40] and [41] we have simulated the two-dimensional \( XY \) model at \( \beta = 1.1199 \), which is the best estimate of the inverse KT transition temperature [42], on lattices up to \( L = 4096 \). Fitting the energy density for \( 16 \leq L \leq 4096 \) with the ansatz

\[
E(L) = E(\infty) + cL^{-\epsilon},
\]

where \( E(\infty), c \) and \( \epsilon \) are free parameters, we get \( \epsilon = 1.85(2) \) with \( \chi^2/\text{d.o.f.} \) smaller than 1. Here we do not intend to further discuss this phenomenological observation; i.e. whether this effective exponent is e.g. caused by logarithmic corrections. We have also generated data for the 2D \( XY \) model for various values of \( \beta \) in the range \( \beta_{\text{max}} < \beta \leq \beta_{\text{KT}} \) for various lattice sizes \( L \) with \( L \lesssim 4\xi_{\text{2nd}} \). These data can be nicely fitted with the ansatz (50), where now \( \epsilon \) apparently depends on \( \beta \); it is decreasing with decreasing \( \beta \). For example, for \( \beta = 1.0929 \) we find, fitting the data for \( 16 \leq L \leq 512 \), the effective exponent \( \epsilon = 1.67(2) \). And for \( \beta = 1.0 \), where \( \xi_{\text{2nd}} = 40.09(8) \), we find, fitting the data for \( 16 \leq L \leq 128 \), the effective exponent \( \epsilon = 0.93(1) \).

From these observations in the two-dimensional \( XY \) model we learn that for \( \beta_{\text{max}} < \beta \leq \beta_{\text{KT}} \) the extrapolation to the thermodynamic limit is non-trivial. In order to keep the systematic error small, we simulated lattices that are as large as possible. Since we had only few lattice sizes at hand, and the effective exponent \( \epsilon \) is not known \textit{a priori}, we have also extrapolated our data in the range \( \beta_{\text{max}} < \beta \leq \beta_{\text{KT}} \) using \( \epsilon = 2 \). In order to estimate the systematic error of this extrapolation, we compared results obtained for different \( L \).

In table 5 we have summarized the lattice sizes \( L_0, L = L_1 = L_2 \) and the values of \( \beta \) that we have simulated. Typically we have performed \( 10^3 \) measurements for each simulation. Details are given in table 5. For each measurement we performed one Metropolis sweep, several overrelaxation sweeps, single-cluster and wall cluster updates. Integrated autocorrelation times in units of measurements for the energy density are \( \tau_{E,\text{int}} \lesssim 10 \) for these simulations. Note that in the case of \( L_0 = 32 \) we have skipped the range \( \beta_{\text{max}} \lesssim \beta \lesssim \beta_{\text{KT}} \), since we were not able to simulate sufficiently large \( L \) to get good control on the thermodynamic limit. In total these simulations took about three years of CPU time on a single core of a 2218 Opteron processor (2.60 GHz).

Like for the case of the three-dimensional bulk system in the low temperature phase, we have computed the specific heat by fitting the data for the energy density with the ansatz (34). Also here we have taken our final results from fits with \( n = 4 \). We have adjusted the range of the fit \( \Delta \) such that \( \chi^2/\text{d.o.f.} \) is about 1.

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Table 5. We give a compilation of the simulations that we have performed. In the first column we give the thickness $L_0$ of the film. In the second column we give the 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 the inverse temperature that has been simulated. In the fifth column we give the step size $\Delta \beta$ that has been used. For example, $\beta_{\text{min}} = 0.49$, $\beta_{\text{max}} = 0.52$ and $\Delta \beta = 0.001$ means that $\beta = 0.49, 0.491, 0.492, \ldots, 0.52$ have been simulated. Finally, in the last column we give the number of measurements (Stat) that have been performed for each of the simulations.

| $L_0$ | $L_1 = L_2$ | $\beta_{\text{min}}$ | $\beta_{\text{max}}$ | $\Delta \beta$ | Stat |
|-------|-------------|---------------------|---------------------|----------------|------|
| 8     | 40          | 0.525               | 0.555               | 0.001          | $10^6$ |
| 8     | 64          | 0.49                | 0.52                | 0.001          | $5 \times 10^5$ |
| 8     | 128         | 0.52                | 0.527               | 0.001          | $2 \times 10^5$ |
| 8     | 128         | 0.544               | 0.56                | 0.001          | $2 \times 10^5$ |
| 8     | 256         | 0.528               | 0.537               | 0.001          | $10^5$ |
| 8     | 256         | 0.544               | 0.56                | 0.001          | $10^5$ |
| 8     | 256         | 0.562               | 0.58                | 0.002          | $10^5$ |
| 8     | 512         | 0.5375              | 0.548               | 0.0005         | $10^5$ |
| 8     | 512         | 0.549               | 0.56                | 0.001          | $10^5$ |
| 8     | 512         | 0.562               | 0.58                | 0.002          | $10^5$ |
| 8     | 1024        | 0.5435              | 0.548               | 0.0005         | $10^5$ |
| 8     | 2048        | 0.545               |                     |                | $14 \times 10^4$ |
| 16    | 128         | 0.49                | 0.4995              | 0.0005         | $10^5$ |
| 16    | 256         | 0.527               | 0.550               | 0.001          | $2 \times 10^5$ |
| 16    | 512         | 0.500               | 0.512               | 0.001          | $10^5$ |
| 16    | 512         | 0.5125              | 0.529               | 0.0005         | $10^5$ |
| 16    | 512         | 0.53                | 0.55                | 0.001          | $10^5$ |
| 16    | 1024        | 0.521               | 0.529               | 0.0005         | $10^5$ |
| 16    | 1600        | 0.5223              |                     |                | $10^5$ |
| 16    | 1800        | 0.522               | 0.523               | 0.00025        | $5 \times 10^4$ |
| 32    | 256         | 0.49                | 0.505               | 0.0005         | $10^5$ |
| 32    | 256         | 0.50525             | 0.50875             | 0.00025        | $10^5$ |
| 32    | 256         | 0.516               | 0.518               | 0.0002         | $10^5$ |
| 32    | 256         | 0.5185              | 0.526               | 0.0005         | $10^5$ |
| 32    | 512         | 0.509               | 0.5128              | 0.0002         | $2 \times 10^5$ |
| 32    | 512         | 0.516               | 0.518               | 0.0002         | $10^5$ |
| 32    | 512         | 0.5185              | 0.526               | 0.0005         | $10^5$ |
| 32    | 1024        | 0.513               | 0.5136              | 0.0002         | $5 \times 10^4$ |

In the case of $L_0 = 8$ we have used in the neighbourhood of the maximum of the specific heat $\Delta = 0.003$. As we go away from the maximum $\Delta$ is increased up to $\Delta = 0.011$ for the smallest and largest values of $\beta$ that we have simulated.

In figure 3 we plot results for the specific heat for $L_0 = 8$ in the most difficult range of $\beta$ around the maximum of the specific heat. With this plot we wish to check two sources of systematic error. First we investigate the truncation effects of equation (34). To this end we have plotted the results obtained with $n = 3$ in addition to those obtained with $n = 4$. Second we investigate systematic errors of the extrapolation to the two-dimensional thermodynamic limit in the range $\beta_{\text{max}} < \beta \leq \beta_{\text{KT}}$. To this end we have replaced the
Figure 3. In the figure we give results for the two-dimensional thermodynamic limit of the specific heat defined by equation (11) for films of the thickness $L_0 = 8$. These results were obtained by fitting our data for the energy density with the ansatz (34) using $n = 3$ and 4. We have used two different sets (set 1, set 2) of data for the energy density. For a detailed discussion see the text. Note that $\beta_{KT} = 0.549278(5)$ [9] for $L_0 = 8$, while the maximum of the specific heat is located at $\beta \approx 0.5432$ as we read off from the plot. Furthermore we show the specific heat computed by using (12) for $L_1 = L_2 = 40$. Deviations from the two-dimensional thermodynamic limit are clearly visible. The peak is less sharp and the maximum is shifted to $\beta \approx 0.539$.

values for the energy density obtained from the extrapolation of $L = 512$ and 1024 (set 1) with those obtained from the extrapolation of $L = 256$ and 512 (set 2).

The results obtained from $n = 3$ and 4 fall nicely on top of each other. Hence there should be no systematic errors due to the truncation of equation (34) that are considerably larger than the statistical error. On the other hand, comparing the results obtained from set 1 and set 2 we see discrepancies that are a few times the statistical error. Note that this problem affects only the range $\beta_{\text{max}} < \beta \leq \beta_{KT}$. The statistical error of the specific heat is maximal at the peak of the specific heat. There it is about 0.01. Instead, computing the specific heat by using equation (12) we get e.g. for $\beta = 0.543$, $L = 512$ the result $C = 12.52(9)$, for $\beta = 0.5435$, $L = 512$ the result $C = 12.62(9)$ and for $\beta = 0.5435$, $L = 1024$ the result $C = 12.48(11)$. That is, the values for the specific heat are compatible with those obtained by fitting the energy density; however the statistical error is about ten times larger.

In the study of the standard $XY$ model with free boundary conditions [20] lattices with $L = L_1 = L_2 = 5L_0$ have been used. Also in the study of the standard $XY$ model with staggered boundary conditions [18,19] only lattices up to $L = 100$ have been used. The authors argue, on the basis of the comparison of results for different values of $L$, 

\[ \text{doi:10.1088/1742-5468/2009/10/P10006} \]
that this is sufficient at the level of their accuracy. Therefore, in figure 3 we also give results for \( L = 5 \times 8 = 40 \). For simplicity we have computed these results by using equation (12), where the statistics is about ten times larger than that of most of the simulations discussed above. At the level of our statistical accuracy, deviations from the two-dimensional thermodynamic limit become clearly visible: the peak of the specific heat is less sharp, the maximum is shifted to \( \beta_{\text{max}} \approx 0.539 \) and its value is lowered to \( C_{\text{max}} \approx 12.1 \). Also the shape of the peak is different: it is steeper for \( \beta < \beta_{\text{max}} \) and on the other hand quite shallow for \( \beta > \beta_{\text{max}} \).

In the case of \( L_0 = 16 \) we have used in the neighbourhood of the peak of the specific heat \( \Delta = 0.001 \) for the fits of the energy density. As we go away from the maximum, \( \Delta \) is increased up to \( \Delta = 0.015 \) for the smallest and largest values of \( \beta \) that we have simulated. At the maximum of the specific heat the statistical error is about 0.01. The ratio \( L/L_0 \) that we have maximally reached for \( L_0 = 16 \) is smaller than for \( L_0 = 8 \). It is comparable with that of the data included into set 2 for \( L_0 = 8 \) discussed above. Therefore we expect deviations from the two-dimensional thermodynamic limit in the range \( \beta_{\text{max}} < \beta \lesssim \beta_{\text{KT}} \) to be of similar size to those for set 2, i.e. a few times the statistical error that we have reached. Note again that outside of this interval, the two-dimensional thermodynamic limit is well under control.

In the case of \( L_0 = 32 \) we did not study the range \( \beta_{\text{max}} < \beta \lesssim \beta_{\text{KT}} \), since we could not simulate sufficiently large lattices to get a good approximation of the two-dimensional thermodynamic limit. For the \( \beta \)-values closest to the peak of the specific heat, we have used \( \Delta = 0.0015 \). For our largest and smallest values of \( \beta \) we have used \( \Delta = 0.015 \). Close to the peak the statistical error of \( C \) is about 0.01.

In figure 4 we have plotted our results for the specific heat for the three-dimensional bulk system and the thicknesses \( L_0 = 8, 16 \) and 32.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{We plot our results for the specific heat as a function of the inverse temperature \( \beta \). In addition to the 3D bulk specific heat we give our results for the thicknesses \( L_0 = 8, 16 \) and 32.}
\end{figure}
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Figure 5. We plot $[C_{\text{bulk}}(\beta) - C(\beta, L_0)]L_0^{-\alpha/\nu}$ as a function of $L_0/\xi_{2nd}(\beta)$ for the thicknesses $L_0 = 8, 16$ and $32$. For a discussion see the text.

The position of the peak of the specific heat approaches the transition temperature of the three-dimensional bulk system and the height of the peak increases as the thickness $L_0$ of the film increases. It is interesting to note that in the case of $L_0 = 8$ for low temperatures the specific heat of the film is larger than for the bulk system, while for $L_0 = 32$ it is smaller. The specific heat of the films at the maximum is larger than the bulk specific heat.

5. Results for the finite size scaling function $f_2$

In this section we compute the finite size scaling function $f_2$ using the numerical data for the specific heat discussed above. Our results are compared with those obtained from experiments on films of $^4$He near the $\lambda$-transition and with results obtained by using field theoretic methods.

5.1. The high temperature phase

First we compute $f_2$ without taking into account corrections. To this end, in figure 5, we have plotted $[C_{\text{bulk}}(\beta) - C(\beta, L_0)]L_0^{-\alpha/\nu}$ as a function of $L_0/\xi_{2nd}(\beta)$, where $\xi_{2nd}(\beta)$ is given by equation (17). Corrections are clearly visible. Note that for the whole range of $L_0/\xi_{2nd}(\beta)$ that is plotted, the error of $[C_{\text{bulk}}(\beta) - C(\beta, L_0)]$ should be at most 0.01. That is, the error is much smaller than the difference between the results obtained for different $L_0$.

Next, in figure 6, we have taken into account boundary corrections by replacing $L_0$ by $L_{0,\text{eff}} = L_0 + L_s$ with $L_s = 1.02$. This has two effects: on the $x$-axis we replace $L_0/\xi_{2nd}$ by $L_{0,\text{eff}}/\xi_{2nd}$ and secondly, in order to compute the energy density, we replace the volume $L_0L_1L_2$ by the effective volume $L_{0,\text{eff}}L_1L_2$. Hence the specific heat that we have computed...
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Figure 6. We plot $[C_{\text{bulk}}(\beta) - C(\beta, L_0)/L_0/\xi_{2nd}]^{\alpha/\nu}$ as a function of $L_0/\xi_{2nd}(\beta)$ for the thicknesses $L_0 = 8, 16$ and 32. For a discussion see the text.

Table 6. We give our results for $f_2$ obtained from $L_0 = 32$ and corrections characterized by $L_s = 1.02$ and $w = 3.5$ for a few values of $L_0/\xi_{2nd}$ (upper row). Using instead $L_s = 1.02$ and $w = 0$, the value of $f_2$ is smaller by about 0.11 throughout.

| $L_0/\xi_{2nd}$ | 0.8 | 0.9 | 1.0 | 1.1 | 1.2 | 1.3 | 1.4 | 1.5 | 1.6 | 1.7 | 1.8 | 1.9 | 2.0 |
|------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|                  | 4.52| 4.17| 3.88| 3.62| 3.39| 3.19| 3.00| 2.84| 2.69| 2.56| 2.43| 2.32| 2.21|

before is multiplied by $L_0/L_0/\xi_{2nd}$. Now the corrections are much reduced in comparison with figure 5. In particular the curves for $L_0 = 16$ and 32 fall almost on top of each other.

Finally, in figure 7, we have taken into account corrections due to possible boundary effects on the analytic background by adding the term $w/L_0/\xi_{2nd}$. The curves match only marginally better than in figure 6. Note that while in the case of figure 6 the value of $f_2$ was increasing with increasing $L_0$, it is decreasing in the case of figure 7. Therefore it seems to be reasonable to assume that the asymptotic result for $f_2$ is located between $[C_{\text{bulk}}(\beta) - C(\beta, L_0)/L_0/\xi_{2nd}]^{\alpha/\nu}$ and $[C_{\text{bulk}}(\beta) - C(\beta, L_0)/L_0/\xi_{2nd} + w/L_0/\xi_{2nd}]^{\alpha/\nu}$ with $w = 3.5$.

In table 6 we give $f_2$ for a few values of $L_0/\xi_{2nd}$. This should help the reader to compare our result with those obtained from other systems.

In figure 8 we plot $[C_{\text{bulk}}(t) - C(t, L_0)]^{\alpha/\nu}$ as a function of $L_0/\xi_{2nd}(t)$ using the experimental data of [43, 44] for thin films of $^4$He at vapour pressure of the thicknesses 483, 1074, 2113, 5039, 6918 and 9869 Å. These data are taken from the web page [45]. The experimental data for the specific heat are given as a function of the reduced temperature $t = (T - T_{\lambda})/T_{\lambda}$. In order to plot them as a function of $L_0/\xi_{2nd}(t)$ we use $\xi_{2nd} = 1.422|t|^{-\nu}$ Å, equation (41). As value of the critical exponents we take

\begin{align*}
\alpha &= 0.76,
\nu &= 0.68,
\gamma &= 1.5,
\delta &= 1.0,
\end{align*}

where $\gamma$ and $\delta$ are the critical exponents for the specific heat and the susceptibility, respectively.
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Figure 7. In the figure we plot $[C_{\text{bulk}}(\beta) - C(\beta, L_0)/L_{0,\text{eff}} + w/L_{0,\text{eff}}]L_0^{-\alpha/\nu}$ with $w = 3.5$ as a function of $L_{0,\text{eff}}/\xi_{2\text{nd}}(\beta)$ for the thicknesses $L_0 = 8, 16$ and 32. For a discussion see the text.

$\nu = 0.6717$ [22] and correspondingly $\alpha = -0.0151$. Furthermore we plot the results of [46] for a film of 57 $\mu$m thickness. The numbers [47] used for the plot are those of [11] plotted in figure 29. We have replaced $x = tL_0^{1/\nu}$ by $L_0/\xi_{2\text{nd}}$ on the $x$-axis and have multiplied $f_2$ by a factor $57,000^{0.0151/0.6717 - 0.0127/0.6709} = 1.04$. Note that the authors of [11] assume $\nu = 0.6709$ [36], while we prefer $\nu = 0.6717$ [22].

For comparison we give our result for $f_2$ obtained from $L_0 = 32$, taking into account boundary corrections characterized by $L_a = 1.02$ and $w = 3.5$ (solid black line). To indicate the possible error we give in addition the result obtained for $L_0 = 32$, $L_a = 1.02$ and $w = 0$ (dashed black line). We have multiplied our numbers by $r_{4\text{He},\phi^+} = 2.57$, equation (45).

We observe that $f_2$ computed from the specific heat of 483, 1074 and 2113 Å films is systematically larger than our result. In contrast, we see a quite good match with the results obtained from 5039 and 6918 Å and (a little worse) for 9869 Å films. Also in the case of the 57 $\mu$m film we see a reasonable match with our result. Note that there are experimental results available for much larger and for smaller values of $L_0/\xi$ than are plotted in figure 8.

The scaling function $f_2$ has been calculated perturbatively to one-loop order in three dimensions, fixed [15, 16]. Also in this case, the relative factor between the experimental and theoretical results for the specific heat was fixed by using the behaviour of the specific heat in the thermodynamic limit. To this end the experimental data of [48] were used. In [15] the result for $f_2$ is only given as log–log plot. Therefore we refrain from plotting it in figure 8. For example, in figures 29 and 31 of [11] the field theoretic result of [15] is plotted along with the experimental results of [36]. There is a quite reasonable match between the field theoretic result and the experimental data. For $tL_0^{1/\nu} \lesssim 12$, the experimental result for $f_2$ is somewhat larger than that of [15]. To pick out one point: for $tL_0^{1/\nu} = 1$ we
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Figure 8. Experimental results [43, 44, 46] obtained for films of $^4$He in the high temperature phase, close to the $\lambda$-transition. We plot $[C_{\text{bulk}}(t) - C(t, L_0)]L_0^{-\alpha/\nu}$ as a function of $L_0/\xi_{2\text{nd}}(t)$ for the thicknesses $L_0 = 483, 1074, 2113, 5039, 6918, 9869$ Å and $57 \mu$m. For comparison we give our results obtained for $L_0 = 32$. In contrast to the experimental results case, boundary corrections, characterized by $L_s = 1.02$ and $w = 3.5$ (solid black line) or by $L_s = 1.02$ and $w = 0$ (dashed black line), are taken into account. Furthermore we have multiplied our results for $f_2$ by $r_{^4\text{He},\phi^*} = 2.57$. For a discussion see the text.

read off from figure 31 of [11] for [15] the value $f_2 \approx 10$. This has to be compared with our result $f_2(\xi_{2\text{nd}}/L_0 = 1/1.422) = 12.6(1)$, where the factor $r_{^4\text{He},\phi^*} = 2.57$ has been taken into account. In equation (8.1) of [13] the specific heat of the thin film has been calculated up to $O(\epsilon)$ as a function of $L_0/\xi_{2\text{nd}}$. Here we refrain from evaluating this function. In section 4.3 we have discussed the case $L_0/\xi_{2\text{nd}} = 0$. Below, in section 5.4, we shall discuss the limits $L_0/\xi_{2\text{nd}} \rightarrow \infty$ and $L_0/\xi_T \rightarrow \infty$.

5.2. The low temperature phase

Next we did the same exercise using our data in the low temperature phase. First we compute the finite size scaling function $f_2$ without taking into account corrections. To this end, in figure 9, we have plotted $[C_{\text{bulk}}(\beta) - C(\beta, L_0)]L_0^{-\alpha/\nu}$ as a function of $L_0/\xi_T(\beta)$, where $\Upsilon(\beta) = 1/\xi_T(\beta)$ is given by equation (20). As in the high temperature phase, scaling corrections are clearly visible. Deep in the low temperature phase, the function even changes sign as the thickness $L_0$ of the film increases. Note that these differences are clearly larger than the statistical errors. As we have discussed before, the error of $[C_{\text{bulk}}(\beta) - C(\beta, L_0)]$ should be at most 0.01 outside of the interval $\beta_{\text{max}} < \beta < \beta_{\text{KT}}$ and may be up to 0.05 inside of this interval. This almost directly translates into the error of $[C_{\text{bulk}}(\beta) - C(\beta, L_0)]L_0^{-\alpha/\nu}$ since $L_0^{-\alpha/\nu}$ is close to 1 for $L_0 = 8, 16$ and 32.

In figure 10 we have taken into account the leading corrections to the singular part of the specific heat by replacing $L_0$ by $L_{0,\text{eff}} = L_0 + L_s$. This has two effects. On the
We plot $[C_{\text{bulk}}(\beta) - C(\beta, L_0)]L_0^{-\alpha/\nu}$ as a function of $L_0/\xi_T(\beta)$ for the thicknesses $L_0 = 8, 16$ and 32. For a discussion see the text.

Figure 10. We plot $[C_{\text{bulk}}(\beta) - C(\beta, L_0)L_0/L_{0,\text{eff}}]L_{0,\text{eff}}^{-\alpha/\nu}$ as a function of $L_{0,\text{eff}}/\xi_T(\beta)$ for the thicknesses $L_0 = 8, 16$ and 32. For a discussion see the text.

In figure 11 we have taken into account the correction $w/L_{0,\text{eff}}$, where we have set $w = 3.5$. Now the curves fall nicely on top of each other giving support to the

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Figure 11. We plot $[C_{\text{bulk}}(\beta) - C(\beta, L_0) L_0 / L_{0,\text{eff}} + w / L_{0,\text{eff}}] L_{0,\text{eff}}^{-\alpha/\nu}$ with $w = 3.5$ as a function of $L_{0,\text{eff}} / \xi_T(\beta)$ for the thicknesses $L_0 = 8, 16$ and $32$. For a discussion see the text.

Table 7. We give $f_2$ for a few values of $L_{0,\text{eff}} / \xi_T$ (upper row). These numbers are obtained from $L_0 = 32$ and corrections characterized by $L_s = 1.02$ and $w = 3.5$. Assuming $L_s = 1.02$ and $w = 0$, the values of $f_2$ are lower by about 0.11 throughout.

| $L_{0,\text{eff}} / \xi_T$ | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 | 1.1 | 1.2 | 1.3 | 1.9 | 2.0 | 2.5 |
|--------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|                          | 11.75 | 10.67 | 9.66 | 8.67 | 7.64 | 6.54 | 5.33 | 3.98 | 2.50 | 0.96 | 1.11 | 1.08 | 0.97 |

Table 8. We give $f_2$ for a few values of $L_{0,\text{eff}} / \xi_T$ (upper row). These results are obtained from $L_0 = 16$ and corrections characterized by $L_s = 1.02$ and $w = 3.5$. Assuming $L_s = 1.02$ and $w = 0$, the values of $f_2$ are lower by about 0.22 throughout.

| $L_{0,\text{eff}} / \xi_T$ | 1.4 | 1.5 | 1.6 | 1.7 | 1.8 |
|--------------------------|-----|-----|-----|-----|-----|
|                          | −0.22 | −0.25 | 0.67 | 0.94 | 1.02 |

suggestion made in section 3 that boundary corrections to the analytic background are not well described by replacing $L_0$ by $L_{0,\text{eff}} = L_0 + L_s$. Note that now the uncertainty of $w$ gives the largest contribution to the error of $[C_{\text{bulk}}(\beta) - C(\beta, L_0) L_0 / L_{0,\text{eff}} + w / L_{0,\text{eff}}] L_{0,\text{eff}}^{-\alpha/\nu}$.

In tables 7 and 8 we give $f_2$ for a few values of $L_{0,\text{eff}} / \xi_T$. This should help the reader to compare our result with those obtained from other systems.

The finite size scaling function shows a clear minimum at a finite value of $[L_{0,\text{eff}} / \xi_T]$. By construction, the position of this minimum does not depend on $w$. For $L_0 = 16$ we get $[L_{0,\text{eff}} / \xi_T]_{\text{min}} \approx 1.452$. For $w = 3.5$ the minimum takes the value $-0.47$ and for $w = 0$ the
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Figure 12. Experimental results [43, 44, 46] obtained for films of $^4$He in the low temperature phase, close to the $\lambda$-transition. We plot $[C_{\text{bulk}}(t) - C(t, L_0)]L_0^{-\alpha/\nu}$ as a function of $L_0/\xi_T(t)$ for the thicknesses $L_0 = 483, 1074, 2113, 5039, 6918, 9869$ Å and 57 μm. For comparison we give our results obtained for $L_0 = 16$ and 32. In contrast to the experimental results case, boundary corrections, characterized by $L_s = 1.02$ and $w = 3.5$ (solid black lines) or by $L_s = 1.02$ and $w = 0$ (dashed black lines), are taken into account. Our results for $f_2$ are multiplied by $r_{^4\text{He},\phi^4} = 2.57$. For a discussion see the text.

value $-0.69$. For $L_0 = 8$ we get $[L_{0,\text{eff}}/\xi_T]_{\min} \approx 1.468$ and the values $-0.36$ for $w = 3.5$ and $-0.76$ for $w = 0$. We consider it as a robust result that $f_2$ assumes a negative value at its minimum. Note that the KT transition takes place at $L_0/\xi_T = 1.595(7)$ [10]. That is, the minimum of $f_2$ is located at a temperature slightly higher than the transition temperature.

In figure 12 we compare our result for $f_2$ with experimental ones. To this end, we plot $[C_{\text{bulk}}(t) - C(t, L_0)]L_0^{-\alpha/\nu}$ as a function of $L_0/\xi_T(t)$ using the experimental data of [43, 44] for thin films of $^4$He at vapour pressure of the thicknesses 483, 1074, 2113, 5039, 6918 and 9869 Å. These data are taken from the web page [45]. The experimental data for the specific heat are given as a function of the reduced temperature $t = (T - T_\lambda)/T_\lambda$. In order to plot them as a function of $L_0/\xi_T(t)$ we use $\xi_T = 3.45 |t|^{-\nu}$ Å, equation (40). As values of the critical exponents we take $\nu = 0.6717$ [22] and correspondingly $\alpha = -0.0151$. Furthermore we plot the results of [46] for a film of 57 μm thickness. We have rescaled these data as discussed in the previous subsection on the high temperature phase. For comparison we give our result for $f_2$ obtained from $L_0 = 16$ and 32, taking into account boundary corrections characterized by $L_s = 1.02$ and $w = 3.5$ (solid black lines). To indicate the possible errors we give in addition the results obtained for $L_s = 1.02$ and $w = 0$ (dashed black lines). We have multiplied our numbers by $r_{^4\text{He},\phi^4} = 2.57$, equation (45).

Here almost all experimental results for the finite size scaling function $f_2$ are somewhat larger than ours. There is some scattering among the experimental results. Those for the

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larger thicknesses of the film are closest to our $f_2$. There is a nice match for the position of the minimum of $f_2$ obtained from 57 $\mu$m and our result. However, $f_2$ computed by using the experimental data never assumes negative values. Also the dip around the minimum is much less pronounced than it is in our case. It is beyond the scope of the present work to discuss possible sources of these discrepancies. This requires detailed discussions with the experimentalists.

5.3. The finite size scaling function $f_2$ in the neighbourhood of the critical point

Here we would like to give an explicit formula for $f_2$ in the neighbourhood of $t = 0$. To this end, we use the results for the amplitudes $A_{\pm}$ obtained in section 4.1, the amplitudes of the correlation length $\xi_{0,2nd}$ and $\xi_{0,T}$ and the value of $f_2(0)$ obtained in section 4.3. In addition we have extracted from our data the slope of the specific heat for thin films at the transition temperature of the three-dimensional bulk system.

As result we get in the high temperature phase

$$f_2 = 161.6(6) - 2.1\delta - [158.3(6) - 2\delta](L_0/\xi_{2nd})^{-\alpha/\nu} + 0.65(2)(L_0/\xi_{2nd})^{1/\nu} + \cdots,$$

(51)

where $\delta = 1/\alpha + 1/0.0151$ gives the dependence on the value of $\alpha$ that is used for the analysis. This formula gives a good approximation of $f_2$ up to about $L_0/\xi_{2nd} = 0.7$, where the deviation from the full result as computed above is less than 1%.

In the low temperature phase we obtain

$$f_2 = 161.6(6) - 2.1\delta - [152.2(6) - 2\delta](L_0/\xi_T)^{-\alpha/\nu} - 2.43(5)(L_0/\xi_T)^{1/\nu} + \cdots.$$

(52)

This is a good approximation of $f_2$ up to about $L_0/\xi_T = 0.3$, where the deviation from the full result as computed above is less than 1%.

5.4. The finite size scaling function $f_2$ for large $|t|$

In the high temperature phase, for $L_0 \gg \xi_{2nd,3D}$, the two boundaries are uncorrelated and therefore the dependence of physical quantities on $L_0$ is trivial. In the case of the specific heat we can write (ignoring boundary corrections)$^7$

$$L_0 C(\beta, L_0) = L_0 C_{\text{bulk}}(\beta) + 2C_s(\beta) \quad \text{for} \quad \beta < \beta_c, \quad L_0 \gg \xi_{2nd,3D}. \quad (53)$$

Inserting this equation in the definition of the scaling function $f_2$ we get

$$f_2 = -2C_s(\beta)L_0^{-1-\alpha/\nu} \quad \text{for} \quad L_0 \gg \xi_{2nd,3D}. \quad (54)$$

Since $f_2$ is a function of $L_0/\xi_{2nd}$ only and $C_s(\beta)$ does not depend on $L_0$, it follows that

$$C_s = h_+\xi_{2nd}^{1+\alpha/\nu}. \quad (55)$$

Following the convention in the literature,

$$h_+ = \frac{A^+_{\xi_{0,2nd}}}{\alpha + \nu}. \quad (56)$$

We do not have data for a sufficiently large range of temperatures to check this behaviour carefully. Assuming the correctness of equation (54) we read off from our data

$^7$ In the low temperature phase, due the Goldstone mode, there should be power like corrections to this behaviour.

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\[
h_+ = -2.2(2) \tag{57}
\]
in the high temperature phase and
\[
h_- = -1.2(2) \tag{58}
\]
in the low temperature phase, where
\[
h_- = \frac{A_s^+ \xi_{0,T}^{-1-\alpha/\nu}}{\alpha + \nu}. \tag{59}
\]
In both cases, we have taken into account the boundary corrections. It follows that \( A_s^+ = -5.2(5) \) and \( A_s^- = -6.8(1.1) \) in units of J \( \text{Å} \text{mol}^{-1} \text{K}^{-1} \). Furthermore, we can compute the universal ratio
\[
Q = \frac{A_s^+}{A_s^-} = 0.8(2). \tag{60}
\]
Experimental results for films of \(^4\text{He}\) have been summarized by the authors of [12] as
\[
A_s^+ = -5.9 \pm 0.2, \quad A_s^- = -8.6 \pm 0.5 \tag{61}
\]
in units of J \( \text{Å} \text{mol}^{-1} \text{K}^{-1} \). It follows that
\[
Q = \frac{A_s^+}{A_s^-} = 0.69(5). \tag{62}
\]
Our result for \( A_s^+ \) is consistent with that from experiments. In the case of \( A_s^- \) we see a small discrepancy. The results for \( Q \) are consistent within the error bars.

The surface specific heat has been calculated using the perturbative expansion in three dimensions fixed in the two-loop approximation by Mohr and Dohm [49,50]. Inserting numerical values into equations (3), and (4) one gets \( A_s^+ = -5.429 \) and \( A_s^- = -1.822 \) in units of J \( \text{Å} \text{mol}^{-1} \text{K}^{-1} \) [51]. We notice that the value for \( A_s^+ \) is in excellent agreement with our result and also close to the experimental one. In contrast, the value for \( A_s^- \) is clearly ruled out by us as well as by the experiment. Already the authors of [49] have pointed out that their result for \( A_s^- \) does not provide an accurate numerical estimate.

Krech and Dietrich quote as a result of the \( \epsilon \)-expansion, equation (E6) of [13],
\[
A_s^+ \xi_{0,+}^{-1} = -\frac{N}{256\pi} \left\{ 2 + \epsilon \left[ 2 + \ln \pi - \gamma + \frac{N + 2}{N + 8} \right] + O(\epsilon^2) \right\}. \tag{63}
\]
Inserting \( N = 2 \) one gets
\[
A_s^+ \xi_{0,+}^{-1} = -0.0049736 - 0.0073796 \epsilon + \cdots. \tag{64}
\]
In order to compare with the experiments on superfluid \(^4\text{He}\) at vapour pressure we insert \( \xi_{0,+} = 1.422 \) \( \text{Å} \) and then convert from units of \( \text{Å}^{-2} \) to J \( \text{Å} \text{mol}^{-1} \text{K}^{-1} \). We arrive at
\[
A_s^+ = [-1.88 - 2.79 \epsilon + \cdots] J \text{Å} \text{mol}^{-1} \text{K}^{-1}. \tag{65}
\]
Following Eisenriegler [52],
\[
\frac{A_s^+}{A_s^-} = \frac{\pi}{23/2} \frac{N}{N + 8} \epsilon + O(\epsilon^2) = 0.222 \epsilon + O(\epsilon^2), \tag{66}
\]
where we have inserted \( N = 2 \). The result of Eisenriegler has been extended by Upton [53] to \( O(\epsilon^2) \). For \( N = 2 \) one gets
\[
\frac{A_s^+}{A_s^-} = 0.222 \epsilon [1 + 0.93 \epsilon + \cdots]. \tag{67}
\]
For a detailed discussion of the field theoretic results see the PhD thesis of Mohr [50].

\[ \text{doi:10.1088/1742-5468/2009/10/P10006} \]
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6. The finite size scaling function \(f_1\)

In order to compute the finite size scaling function \(f_1\) we have to determine the specific heat at the temperatures where \(\xi_{2nd}\) for the three-dimensional bulk system assumes the values 8, 16 and 32 or, taking into account corrections, 9.02, 17.02 and 33.02. To this end, we have first numerically inverted equation (17). The corresponding values of \(\beta\) are 0.50295, 0.50694, 0.50836 and 0.50396, 0.50713, 0.50840, respectively. At these values of \(\beta\) the specific heat of the three-dimensional bulk system assumes the values 7.091(2), 9.277(2), 11.512(4) and 7.462(2), 9.475(2), 11.613(4), respectively. These values are obtained by using the results of fits with the ansatz (29). The error is dominated by the uncertainty of \(C_{ns}\) that has been used as input in equation (29).

In figure 13 we plot \([(L_0/L_{0,eff})C(t, L_0) - C_{bulk}(t_0) - w/L_{0,eff}]L_{0,eff}^{-\alpha/\nu}\) as a function of \(t(L_{0,eff}/\xi_{0,2nd})^{1/\nu}\), where we have used \(L_s = 1.02\) and \(w = 3.5\). For a discussion see the text.

\[\begin{align*}
\text{Figure 13.} \quad & \text{We plot } [(L_0/L_{0,eff})C(t, L_0) - C_{bulk}(t_0) - w/L_{0,eff}]L_{0,eff}^{-\alpha/\nu} \text{ versus } t(L_{0,eff}/\xi_{0,2nd})^{1/\nu}, \text{where we use } L_s = 1.02 \text{ and } w = 3.5. \text{ For a discussion see the text.}
\end{align*}\]

Now let us compare our result with that from previous Monte Carlo studies. In [18, 19] the function \(f_1\) has been obtained from simulations of the standard \(XY\) model on the simple cubic lattice. The authors have used staggered boundary conditions in order
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Figure 14. We plot $[\langle L_0/L_{0,\text{eff}} \rangle C(t, L_0) - C_{\text{bulk}}(t_0) - 30(\beta_0 - \beta)]L_{0,\text{eff}}^{-\alpha/\nu}$ as a function of $t(L_{0,\text{eff}}/\xi_0)^{1/\nu}$. For a discussion see the text.

...to suppress the order parameter at the boundary. They have simulated lattices of the thicknesses $L_0 \leq 24$ and $L_1 = L_2 \leq 100$. They define the specific heat as the second derivative of the free energy with respect to the temperature. They compute it by using $C = \beta^2[\langle E^2 \rangle - \langle E \rangle^2]/(L_0L_1L_2)$.

In figure 15 we plot the results [54] of [18, 19] along with ours obtained from $L_0 = 16$ and 32 as given in figure 14. To this end, we have multiplied $f_1$ of [18, 19] by $r_{\phi^4,XY} \approx 6.334$. Furthermore in [18, 19] $f_1$ is given as a function of $tL_0^{1/\nu}$ which we have converted into $t(L_0/\xi_0)^{1/\nu}$ here. Some of the data points of [18, 19, 54] are given with an error bar which we have skipped in our figure for better readability. The size of these errors is consistent with the scattering of the data points for different values of $x$. Taking into account the rescaling by $r_{\phi^4,XY}$, the statistical errors of [18, 19] are typically 10–20 times larger than ours. Given these large statistical errors the authors of [18, 19] were not able to conduct an analysis of corrections to the finite size scaling behaviour. Here we should note that in the case of the $XY$ model also corrections $\propto L_0^{-\omega}$ with $\omega = 0.785(20)$ [22] should be present, which complicate the analysis compared with that of the model studied here.

In order to disentangle the effect of a too small ratio $L_1/L_0$ and corrections to scaling which are proportional to some power of $L_0$, we also give in figure 15 results obtained for the $\phi^4$ model with $L_0 = 16$ and $L_1 = L_2 = 5 \times 16 = 80$. Here we took into account the same corrections to scaling as in the case of figure 14. We find that for the choice $L_1/L_0 = 5$ the maximum of $f_1$ is shifted to $x_{\text{max}} \approx -5.8$ compared with $x_{\text{max}} \approx -6.4$ for the limit $L_1/L_0 \to \infty$. Hence the shift of the maximum of $f_1$ of [18, 19] towards higher temperatures can at least partially be explained by a too small choice of $L_1/L_0$. The value $\xi_{0,XY} = 0.4894(5)$ [10] for the standard definition $t = (T - T_c)/T_c$ of the reduced temperature used in [18, 19].
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Figure 15. We plot the results of [18, 19] ($XY$, $L_0 = 12, \ldots, XY$, $L_0 = 24$) and [20] ($XY$, free) for $f_1$ obtained from simulations of the standard $XY$ model on the simple cubic lattice with staggered and free boundary conditions, respectively. The numbers provided by Manousakis [54] correspond to figure 14 of [19] and figure 2 of [20], respectively. We have rescaled the results of [18, 19] and [20] to compare them with ours. In the case of [18, 19] and [20] no corrections to scaling are taken into account; hence $x = t[L_0/\xi_0]^{1/\nu}$ and $f_1 = r_{\phi4,XY}L_0^{-\alpha/\nu}[C(t, L_0) - C_{\text{bulk}}(t_0)]$. For comparison we plot our results obtained from $L_0 = 16$ and 32 as given in figure 14 and in addition results for $L_0 = 16$ and $L_1 = L_2 = 5L_0 = 80$. For a discussion see the text.

of $f_1(x_{\text{max}})$ of [18, 19] is considerably larger than ours. Clearly, this cannot be explained by the effect of a too small $L_1/L_0$. To get a quantitative idea of whether corrections to scaling as discussed above might explain the discrepancy, we have analysed our data for $L_0 = 16$ and $L_1 = L_2 = 5 \times 16 = 80$ in exactly the same fashion as [18, 19] did, not taking into account any corrections to scaling. In this way we find $x_{\text{max}} \approx -5.2$ and $f_1(x_{\text{max}}) \approx 5.5$. These values are indeed very similar to the results found by [18, 19].

The authors of [20] have simulated the standard $XY$ model using films of the thicknesses $L_0 = 12, 14$ and 16. Throughout, they have used $L_1 = L_2 = 5L_0$. They have used free (‘open’ in their notation) boundary conditions in the short direction. Since no clear trend with increasing $L_0$ is visible, we have plotted in figure 15 all data, properly rescaled, using the same symbol. The results of [18, 19] and [20] are consistent, confirming that staggered and free boundary conditions do indeed impose the same boundary conditions on the order parameter. Like in [18, 19], the value of the maximum seems to be larger than in our case; also the position of the peak is shifted slightly towards smaller temperatures. The same discussion as above for [18, 19] should apply.

In figure 16 we compare with experimental results for the finite size scaling $f_1$. In order to compute $t_0$ we have used $\xi_{\text{2nd}} = 1.422 \text{ Å } t^{-0.6717}$, equation (41). We have plotted $[C(t, L_0) - C_{\text{bulk}}(t_0)]L_0^{-\alpha/\nu}$ as a function of $t(L_0/\xi_{0,\text{2nd}})^{1/\nu}$, where the specific heat is given

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Figure 16. We plot $[C(t, L_0) - C_{\text{bulk}}(t_0)]L_0^{-\alpha/\nu}$ as a function of $t(L_0/\xi_0)^{1/\nu}$ for experimental data. For comparison we give our results of figure 14 for $L_0 = 16$ and 32. Our numbers have been multiplied by $r_4^{4\text{He},\phi_4} = 2.57$. For a discussion see the text.

in units of J mol$^{-1}$ K$^{-1}$ and $L_0$ in Å. To this end we have used the data of [43, 44] for thin films of $^4$He at vapour pressure of the thicknesses 483, 2113, 6918 and 9869 Å. These data are taken from the web page [45]. For a better readability of the figure we do not give the data for 1074 and 5039 Å. In addition we give the results of [46]. In this case, we have computed $C_{\text{bulk}}(t_0)$ from the results of the fits given in [36]. For comparison we have taken our results for $L_0 = 16$ and 32 from figure 14. In order to match with the experimental results, we have multiplied our numbers by $r_4^{4\text{He},\phi_4} = 2.57$. In the high temperature phase, the experimental results fall nicely on top of each other. In contrast, in the low temperature phase, in particular for temperatures below the position of the peak, we see some scattering of the experimental results. In the main our results are compatible with those from the experiments on $^4$He films. In the high temperature phase our result is slightly larger than the experimental one.

Finally let us compare our results with those obtained from field theory. In figure 1(a) of [15] a one-loop result for the finite size scaling function $f_1$ is given. The specific heat is given in units of J mol$^{-1}$ K$^{-1}$ and the length in units of Å. The function has similar qualitative features to our result. However the peak in the low temperature phase is much shallower than in our case. The maximal value is about 7, while we get 11.9. The position of the peak ($tL_0^{1/\nu} \approx 9$) slightly differs from ours ($tL_0^{1/\nu} \approx 10.9$).

7. Summary and conclusions

We have studied the finite size scaling behaviour of the specific heat of thin films in the three-dimensional $\chi^3$ universality class. To this end we have simulated the improved two-component $\phi^4$ model on the simple cubic lattice. In order to get a vanishing order
The specific heat of thin films near the $\lambda$-transition parameter at the boundary, which is observed in experiments on films of $^4$He near the $\lambda$-transition, we have employed free boundary conditions. These can be interpreted as Dirichlet boundary conditions with the value $\vec{\phi} = (0,0)$ of the field at the boundary. We discuss how leading boundary corrections affect the finite size scaling behaviour of the specific heat of thin films. We point out that the analytic part of the specific heat might suffer from boundary corrections that are not described by $L_{0,\text{eff}} = L_0 + L_s$, which characterizes the leading corrections to the singular part. 

First we performed simulations to get the energy density of the three-dimensional system for a large number of temperatures. These simulations supplement those of [29,30]. Using these data we computed accurate estimates of the specific heat in the range $0.49 < \beta < 0.58$ of inverse temperatures. 

Next we analysed in detail the finite size scaling behaviour of the specific heat of thin films at the $\lambda$-transition. To this end we have simulated films up to a thickness of $L_0 = 64$ lattice units. Our result is in nice agreement with that obtained for thin films of $^4$He at the $\lambda$-transition [12]. Furthermore we have simulated films of the thicknesses $L_0 = 8, 16$ and 32 for a large range of inverse temperatures $\beta$ in the neighbourhood of the $\lambda$-transition. We have taken great care to obtain reliable estimates for the two-dimensional thermodynamic limit of the thin films. Using our data we have computed the finite size scaling functions $f_1$ and $f_2$ defined in the introduction. It turns out that corrections to scaling which are caused by the free boundary conditions have to be taken into account to get a good collapse of the data obtained for different thicknesses of the film. These corrections can be described, to leading approximation, using an effective thickness $L_{0,\text{eff}} = L_0 + L_s$ of the film. In [10] we have obtained $L_s = 1.02(7)$ from a finite size scaling study at the critical point of the three-dimensional system. However, a priori, this $L_{0,\text{eff}}$ only applies to the singular part of the specific heat. Our analysis of the data shows that in fact the analytic part of the specific heat requires an additional correction which is $\propto L_0^{-1}$. 

The comparison of our results for the finite size scaling functions $f_1$ and $f_2$ and those obtained from experiments on films of $^4$He at the $\lambda$-transition in general show nice agreement. We think that, in order to explain the minor discrepancies, a detailed knowledge of the experimental work is required. Therefore we refrain from any speculation on the sources of these discrepancies.

We have also compared with results obtained from field theory and previous Monte Carlo simulations. Field theoretic calculations are of low order; $O(\epsilon)$ in the case of the $\epsilon$-expansion and one- or two-loop order in the case of the perturbative expansion in three dimensions, fixed. Previous Monte Carlo simulations are affected by relatively large statistical errors. Corrections to finite size scaling were not discussed in these works. 

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