Scaling of the specific heat of superfluids confined in pores

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We investigate the scaling properties of the specific heat of the XY model on lattices $H \times H \times L$ with $L \gg H$ (i.e. in a bar-like geometry) with respect to the thickness H of the bar, using the Cluster Monte Carlo method. We study the effect of the geometry and boundary conditions on the shape of the universal scaling function of the specific heat by comparing the scaling functions obtained for cubic, film, and bar-like geometry. In the presence of physical boundary conditions applied along the sides of the bars we find good agreement between our Monte Carlo results and the most recent experimental data for superfluid helium confined in pores.

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1. Introduction

Bulk liquid ^{4}He exhibits a second order phase transition at the λ-critical temperature $T_\lambda \approx 2.18$K where it turns superfluid. Approaching T_λ from below the specific heat c and the superfluid density have singularities which are characterized by the critical exponents α and ν, respectively; these critical indices determine the universality class of this second order phase transition. If liquid ^{4}He is placed in a confining geometry, e.g. film or pore-like geometry, the finite-size scaling theory[1] can be used to describe the behavior of the physical quantities at temperatures close to T_λ. The finite-size scaling theory is based on the assumption that the system feels its finite size when the correlation length ξ becomes of the order of the confining length. For a

physical quantity O this statement can be expressed as follows:[2]

$$\frac{O(t,H)}{O(t,H=\infty)} = f(x), \quad (1)$$

$$\frac{H}{\xi(t,H=\infty)} = x, \quad (2)$$

where H denotes the relevant confining length and the reduced temperature $t = T/T_\lambda - 1$ while $\xi(t, H = \infty)$ is the correlation length of the bulk system. The point is that the dimensionless function f depends only on the dimensionless ratio H/ξ and it does not depend on microscopic details of the system. It does, however, depend on the type of system, the observable O, the type of confining geometry and on the conditions imposed (or not, in the case of free boundaries) at the boundaries of the system.

Liquid ^{4}He can be an ideal testing ground to check the validity of the finite-size scaling theory experimentally[3] because the specific heat c and the superfluid density can be measured to a very high accuracy. In addition, the shape of the confining geometry, such as films or pores, can be designed with such a precision that the relevant confining length is well defined.

In order to compare the results of finite-size scaling theory with the experimental results on liquid ^{4}He, there have been theoretical efforts to compute the universal finite-size scaling function of the specific heat of confined liquid ^{4}He.[4–10] The scaling function for film geometry has been computed by loop expansion based renormalization group treatment of the standard ϕ^4 Landau-Ginzburg functional[4–7] and by the Monte-Carlo method within the XY model.[8–10] The XY model is another form of the standard Landau-Ginzburg functional and both models belong to the same universality class as liquid ^{4}He, i.e. all three systems have the same critical indices. The scaling functions for a film geometry have been computed from the XY model using the Monte Carlo method[8–10] and they are in rather good agreement with the scaling functions obtained from the field theoretical treatment of the ϕ^4 Landau-Ginzburg theory.[6] The scaling functions obtained when periodic boundary conditions[9] were applied on the top and on the bottom boundary of the film are very different from the scaling functions obtained when staggered boundary conditions[8,10] (vanishing order parameter on the boundary layer) were applied on the top and bottom film boundary. The scaling functions obtained by the Monte Carlo simulation of the XY model[8,10] agree reasonably well with the experimentally determined[3] scaling functions when staggered boundary conditions were applied in the simulation. Such boundary conditions on the order parameter are believed to approximate better the real conditions on the top and bottom boundary of superfluid film.[6,8]

Besides the boundary conditions, the other important factor which, in principle, can determine the scaling function is the geometry. Close enough

to the critical point where the bulk correlation length ξ becomes of the size of the confining length H or even larger, the system as a whole "knows" about the geometrical shape of the confining volume. Thus, one expects to find a region of the dimensionless variable H/ξ where the form of the scaling function is sensitive to the geometry of the confining volume. There are experiments which have been performed for the pore geometry[11–13] and the results for the specific scaling function are significantly different from those obtained from the film geometry. In this paper, we report results of our simulations of the XY model in a bar-like geometry, namely on lattices $H \times H \times L$ with $L >> H$, which mimic the pore-like geometry of the experiments. In addition, to represent the real situation more closely we have used staggered boundary conditions along the confining dimensions (H directions). Periodic boundary conditions are used along the long (L) direction of the bar because they approximate the limit $L \to \infty$ better. We find that our results for the scaling function are different from those obtained for the film geometry and are also in reasonably good agreement with the most recent experimental results[13] without any adjustable parameter.

2. The model

In order to describe the fluctuations of the order parameter in superfluid ^4He near the λ point we employ the XY model which belongs to the same universality class as the Landau-Ginzburg free energy which is expressed in terms of the superfluid order parameter $\psi(\vec{r})$. Within the XY model the free-energy $\mathcal{H}$ can be written as

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j, \tag{3}$$

where the summation is over all nearest neighbors, $\vec{s} = (\cos\theta, \sin\theta)$, and $J > 0$ sets the energy scale. In this model $\vec{s}_i$ are not real spins but they are pseudospin variables[14] in which the angle θ corresponds to the phase of the superfluid order parameter $\psi(\vec{r})$. The order parameter can be understood[14] as the average value of operator which creates an atom in the superfluid helium and it is defined in a volume whose linear extensions are much larger than the interparticle spacing and much smaller than the correlation length, a condition that is realized only very near the transition temperature.

The pore geometry is represented by $H \times H \times L$ lattices with $L \gg H$, namely, bar-like geometry. On the ends of the bar we always use periodic boundary conditions whereas we have carried out separate calculations for a) periodic and b) staggered boundary conditions along the sides (H-directions) of the bar. In the case of staggered boundary conditions the four sides of the

bar are coupled to a staggered pseudospin configuration, i.e. the pseudospins at the boundaries alternate when we move along the lattice bonds (cf. also Ref. [8]) so that the total sum of the spins at the sides of the bars is exactly zero. This boundary condition plays the role of the confining walls and corresponds to a boundary condition where the superfluid order parameter is exactly zero at the boundaries. In the simulation this can be easily visualized by corresponding every spin of the boundary layer to the same pseudospin but which interacts with all other spins of the layer next to the boundary via a coupling which alternates in sign. This spin is a dynamical variable which means that it can change direction during the cluster updating procedure and thus, the $O(2)$ invariance of the model is not broken at the boundaries.

We computed the specific heat on $H \times H \times L$ lattices, where $H = 16, 20, 26, 32$ and $L = 5H$. The specific heat c is obtained by

$$c = \frac{\beta^2}{N} \left(\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 \right), \tag{4}$$

where $\beta = 1/(k_B T)$ and N is the number of pseudospins contributing to the specific heat. The multi-dimensional integrals in the expression for the averages in Eq.(4) were computed by means of the Monte Carlo method using Wolff's 1-cluster algorithm.[15] To thermalize the system, we typically carried out of the order of $20,000$ steps involving single cluster flips during which no observable was calculated. After the end of that process we typically carried out of the order of $750,000$ single cluster flips where observables were calculated. The calculations were performed on several computers of different architechure including IBM RS/6000 and DEC alpha AXP workstations and a Cray Y-MP.

3. Results

Here we check the finite-size scaling hypothesis for the specific heat with respect to the bar diameter H in the $L \to \infty$ limit. We do not need to take the actual $L \to \infty$ limit, because it turns out that lattices with the ratio $L/H = 5$ are a satisfactory approximation to that limit. We demonstrate this in Fig. 1 where the specific heat, calculated on lattices with ratios $L/H = 5, 10, 15$ and $H = 16$, is plotted near the peak. Within error bars the results for the three size lattices are the same.

We are now able to compute the finite-size scaling function $f_1(tH^{1/\nu})$ defined by the expression:[4,5]

$$c(t, H) = c(t_0, \infty) + H^{\alpha/\nu} f_1(tH^{1/\nu}). \tag{5}$$

The function $f_1(x)$ is universal and $\nu = 0.6705$ as has been extracted from recent experiments.[17] The hyperscaling relation $\alpha = 2 - 3\nu$ yields $\alpha/\nu =$

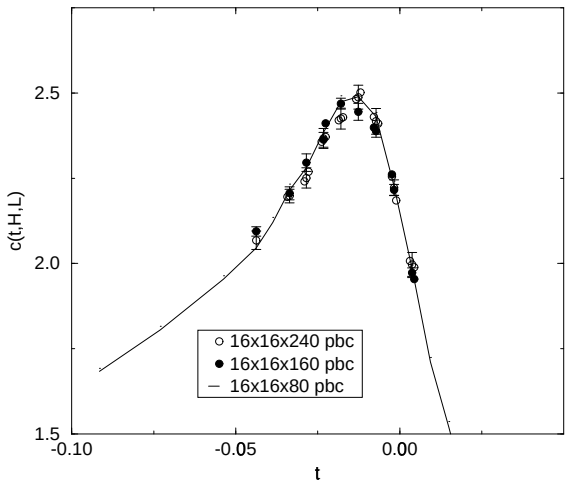

Fig. 1. The specific heat as a function of $t = T/T_\lambda - 1$ for $16^2 \times L$ lattices with periodic boundary conditions (pbc) in all directions. In the three-dimensional XY model $T_\lambda/J = 2.2017$.[16]

-0.0172. At the reduced temperature t_0 the correlation length $\xi(t) = \xi_0^{\pm}|t|^{-\nu}$ becomes equal to the bar thickness H, i.e. $t_0 = (\xi_0^+/H)^{1/\nu}$ with $\xi_0^+ = 0.498$.[18] We have

$$c(t_0, \infty) = c(0, \infty) + \tilde{c}_1^+ t_0^{-\alpha}, \tag{6}$$

where we use the bulk values $c(0, \infty) = 30$, $\tilde{c}_1^+ = -30$ obtained by studying the finite-size scaling of the specific heat of cubes.[9]

There are other choices for universal scaling functions associated with the specific heat which one could make.[9] The reason for making this particular choice is because most of the relevant experimental results have been analyzed using f_1. In general one needs to separate a constant (for example the value of the specific heat at the lambda point) because the singular behavior goes along with the remaining part.

In Fig. 2 we compare the scaling functions $f_1(x)$ for cubes, films (taken from Ref. [9]) and bars in the presence of periodic boundary conditions. The more confining dimensions occur in the system, i.e. one, two, and three confining dimensions for the film, the bar and the cube, respectively, the more the function $f_1(x)$ is suppressed, only in the limit $|x| \to \infty$ do the three functions agree.

Here we compute the scaling function $f_1(x)$ again but using staggered boundary conditions in the H-directions of the lattice. These boundary conditions seem to mimic the physical boundary conditions met in the ex-

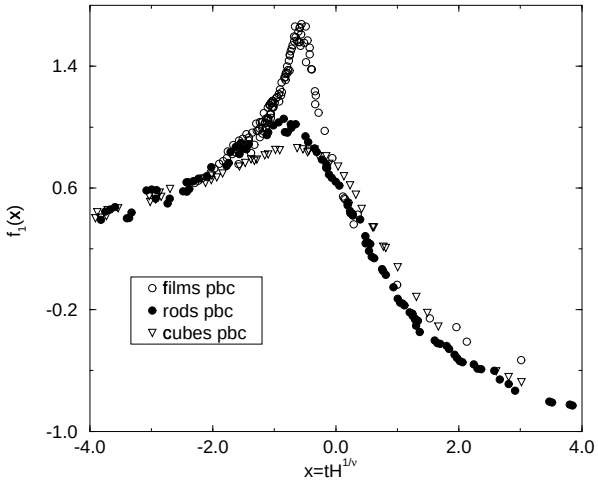

Fig. 2. Comparison of the finite-size scaling functions $f_1(tH^{1/\nu})$ in Eq.(5) for films, bars and cubes with periodic boundary conditions (pbc) in all directions.

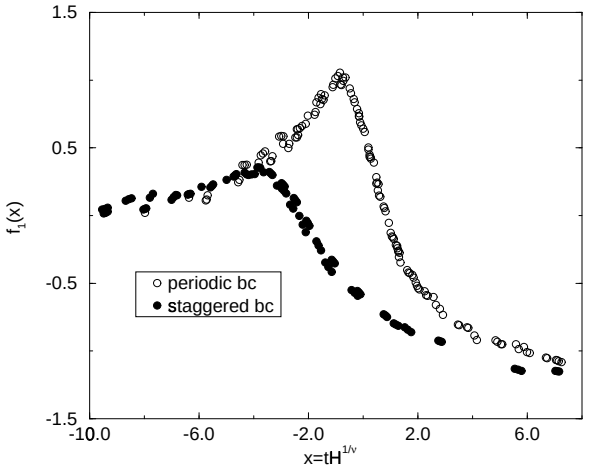

Fig. 3. Comparison of the scaling functions $f_1(x)$ for bars with periodic and staggered boundary conditions on the sides.

periments rather well. This was demonstrated in Ref. [8] where the calculated specific heat scaling function for films agrees reasonably well with the experimental one when such boundary conditions were used and it was very different for periodic boundary conditions. Our results for the scaling function f_1 are shown in Fig. 3 where f_1 is compared to that obtained with periodic boundary conditions. This figure demonstrates that in the presence of staggered boundary conditions the scaling function $f_1(x)$ is dramatically suppressed compared to the function $f_1(x)$ obtained for bar-like geometry with periodic boundary conditions in all directions. For large values of $|x|$ both functions agree. Similar behavior was observed for a film geometry.[8]

In order to relate our results to experimental results let us now compute the finite-size scaling function $f_1(x)$ obtained for bars with staggered boundary conditions in physical units. This leads to the same conversion formula used in Ref. [8]: $f_1(x)|_{phys} = \lambda\, f_1(x)|_{lattice}$ where the factor λ is given by $\lambda = (V_m k_B)/a^3(\text{Å}/a)^{\alpha/\nu}$ where V_m is the molar volume of ^4He at saturated vapor pressure at T_λ. The unit of length a (i.e., the lattice spacing a in the XY model) was determined to be $a = 2.95\text{Å}$[8,9] and thus $\lambda = 15.02 Joule/(^\circ Kmole)$.

Coleman and Lipa[13] have recently measured the specific heat of superfluid helium confined in pore geometry. They have compared their results to the early data of Refs.[11,12]. There is some range of disagreement near the critical temperature. The experimental results of Refs.[11,12] have been obtained on much smaller diameter pores than those of Ref.[13]. In our recent work for the effect of the boundaries on superfluid films[10] we found that the boundary can create corrections to scaling which for films of thickness as large as those of the pore diameters of Refs.[11,12] can not be neglected. Since we want to stay away from such difficulties in this paper, we decided to use the results of the most recent work of Ref.[13] to compare with the results of our theoretical calculations. In Fig. 4 we compare the experimental results reported in Ref.[13] with our Monte Carlo results. Since the authors of Ref.[13] present only their specific heat data we deduced the scaling function $f_1(x)$ according to Eq.(5) using the bulk data of liquid ^{4}He reported in Ref.[19]. The agreement between the theoretical calculation and experiment is satisfactory. Note that the agreement between the function f_1 obtained from Monte Carlo data in the presence of *periodic* boundary conditions in the H-direction and the experimentally determined function f_1 would be far worse. For example, the peak of the function $f_1(x)$ for *periodic* boundary conditions in the H-direction in physical units is about $15 Joule/(^\circ Kmole)$ at $x \approx -4$, whereas for the experimental function $f_1(x)$ is approximately $6.4 Joule/(^\circ Kmole)$) at $x \approx -23.1$ (cf. Fig. 4). The small difference between experimental and theoretical scaling functions obtained

with staggered boundary conditions could be due to a number of reasons, including poor representation of the geometry or the boundary conditions in the real experimental system by the theoretical modeling.

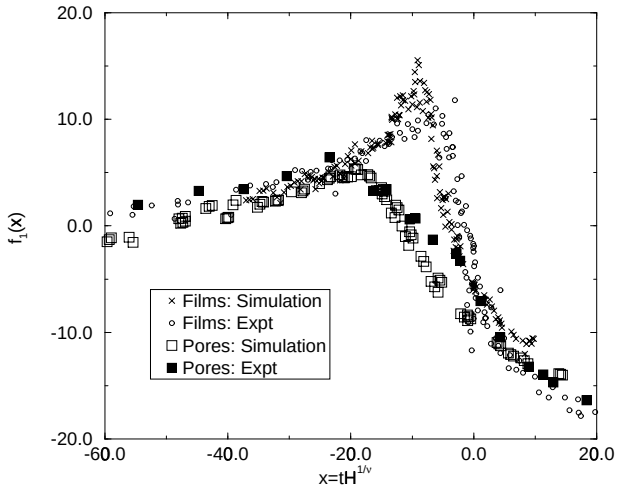

Fig. 4. Our results for the specific heat scaling function $f_1(x)$ for pores (bars) with staggered boundary conditions on the substrate layers (open squares) are compared to the experimental results[13] (solid squares). For comparison the same function is also shown for the film geometry as obtained from our simulation (crosses, taken from Ref. [8]) and from experiments (open circles, taken from Ref. [3]). H is expressed in units of Å and $f_1(x)$ in $Joule/(^\circ Kmole)$.

Fig. 4 demonstrates again the effect of the type of the confining geometry on the shape of the universal scaling function $f_1(x)$, now in the presence of staggered boundary conditions which are a good approximation to the physical boundary conditions imposed by the confining walls.

In conclusion, we have numerically computed the finite–size scaling function $f_1(x)$ for a bar geometry and we have compared our results to the scaling functions obtained earlier for cubes and films. For pores (represented by bars) we find good agreement between our Monte Carlo results in the presence of staggered boundary conditions and the most recent experimental results of Coleman and Lipa.[13] More precise experimental data for the specific heat of liquid ^{4}He confined in pores near the λ-critical temperature T_λ are expected from future experiments[20] which can be compared to our calculation. These experiments could employ different substrates to check the influence of the boundary conditions on the scaling function $f_1(x)$. Thus,

this work together with our earlier work on other geometry[8,10] shows that only scaling functions which belong to the same geometry and the same boundary conditions should be compared.

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