Heat-capacity scaling function for confined superfluids

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We study the specific-heat scaling function of confined superfluids using Monte Carlo simulation. While the scaling function is insensitive to the microscopic details, it depends on the confining geometry and boundary conditions (BC's). In the present work we have studied (a) cubic geometry with open BC's in all three directions and (b) parallel-plate (film) geometry using open BC's along the finite dimension and periodic BC's along the other two dimensions. We find that the specific-heat scaling function is significantly different for the two different geometries studied. The scaling function for each geometry (a) or (b) is very different when compared to that obtained for the same geometry but with periodic BC's. On the contrary, we find that in case (b) the calculated scaling function is very close to the earlier calculated using Dirichlet instead of open BC's. This demonstrates that Dirichlet and open boundary conditions act in a similar way. Our results for both scaling functions obtained for the parallel-plate geometry and for cubic geometry with open BC's along the finite dimensions are in very good agreement with recent very-high-quality experimental measurements with no free parameters.

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I. INTRODUCTION

Thermodynamic quantities such as the specific heat become nonanalytic at a critical point associated with a second-order phase transition. For a finite (or confined) system with a finite dimension such as a film characterized by a length L, close enough to the critical point such that the correlation length becomes comparable or larger than L, such thermodynamic quantities are significantly altered; the reason is that the degrees of freedom of the system are correlated to each other over the entire system. Examples of such confined systems are (a) a film of thickness L where the system is confined in one spatial dimension, (b) a barlike geometry with cross section $L\times L$ and infinite length (such a pore or a wire) where the system is confined in its two spatial dimensions, or (c) a cubic geometry of size L^3 where the system is finite in all three dimensions (3D). For any thermodynamic observable we can define a system specific dimensionless quantity, a scaling function;[1] for example, in the case of the specific heat near the critical point and for sufficiently large L we may define the following scaling function:

$$f(x=tL^{1/\nu})=\frac{c(t,L)-c(0,\infty)}{c(0,L)-c(0,\infty)}, \tag{1}$$

where $t=T/T_\lambda-1$ is the reduced temperature and $c(t,L)$ is the specific heat for the case of the system confined within a finite length L. For a given case of confining geometry and given the condition which the order parameter satisfies at the boundaries of the system, as L approaches infinity and $t\rightarrow 0$, the scaling function depends only on the value of the combination $x=tL^{1/\nu}$—namely, on the length L in units of the correlation length $\xi(t)\sim t^{-\nu}$. A dimensionless function such as $f(x)$ defined by Eq. (1) can be thought of as a universal scaling function for the specific heat for a well-defined confining geometry. In other words, the scaling function does not depend on the microscopic details, but only depends on the nature of the universality class of the system, the confining geometry, and the boundary conditions which are felt by the order parameter.

In this limit ($t\rightarrow 0$ and $L\rightarrow\infty$) the scaling function is different for the three different cases mentioned previously for the following reason: For a fixed value of $x\ll 1$ and for any large value of L there is always a sufficiently small value of t satisfying the condition where the correlation length is much larger than L. However, in this limit case (a) is the case of a 2D plane, case (b) is the case of a 1D line, and case (c) is the zero-dimensional case. Thus the value $f(x)$ for sufficiently small values of $|x|$ should be very different for these three geometries.

Though earlier experiments on superfluid helium films of finite thickness[2] seemed to confirm the validity of the finite-size scaling (FSS), there were later experiments[3,4] where it was shown that the superfluid density of thick helium films does not satisfy FSS when the expected values of critical exponents were used. Similarly, in measurements of the specific heat of helium in finite geometries, other than the expected values for the critical exponents were found.[5]

More recent experiments in microgravity environment[6] as well as Earth-bound experiments[7,8] are consistent with scaling and they have determined the specific-heat scaling function for the parallel plate (film) geometry [case (a)] and they are in reasonable agreement with the scaling function as was predicted by Monte Carlo simulations[9,10] and renormalization group techniques.[11] While the specific-heat scaling function for case (b) confinement has been theoretically determined[12] and it was found to be significantly suppressed relative to case (a) there are so far no experimental data to compare. More recently, the specific-heat scaling function for case (c) has been experimentally determined.[13,14]

The main goal of this paper is to present the results of our Monte Carlo simulations to determine the specific-heat scaling function for cubes with open boundary conditions (BC's) in all three directions [confining case (c)]. In this case the scaling function characterizes the zero-dimensional to three-dimensional transition. Our results for the scaling function are compared to the very recently obtained experimental results for the specific-heat scaling function in the case of cubic confinement.[13,14] We find satisfactory agreement with no free parameters. In addition, we present results for the specific-heat scaling function for the parallel-plate geometry on lattices of size $L_1 \times L_2 \times L$ with $L_1 = L_2 \gg L$ where we have applied periodic BC's along the $L_{1,2}$ directions and open BC's along the film-thickness direction of size L. The latter case was carried out in order to compare the results for *Dirichlet BC's* (vanishing order parameter on the top and bottom of the film) obtained earlier.[9,10] In Refs. 9 and 10 it was found that while the results with periodic BC's along the film-thickness direction were very different from those obtained with Dirichlet BC's, the results obtained with Dirichlet BC's fit the experimental results with no free parameter. In this paper we find that the scaling function obtained with open BC's along a finite dimension is close to that obtained with Dirichlet and also fits reasonably well the experimental results obtained by the so-called confined helium experiment[6] (CHEX).

II. MONTE CARLO CALCULATION

We have performed a numerical study of the scaling behavior of the specific heat of ^{4}He in a cubic and in a film geometry at temperatures close to the critical temperature T_λ. The superfluid transition of liquid ^{4}He belongs to the universality class of the three-dimensional x-y model; thus, we are going to use this model to compute the specific heat at temperatures near T_λ using the cluster Monte Carlo method.[15] The x-y model on a lattice is defined as

$$H = -J \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j , \tag{2}$$

where the summation is over all nearest neighbors, $\vec{s} = (\cos\theta, \sin\theta)$ is a two-component vector which is constrained to be on the unit circle, and J sets the energy scale.

We define the energy density of our model as follows:

$$E = \langle e \rangle = 3 - \frac{1}{V} \left\langle \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j \right\rangle , \tag{3}$$

where $V = L^3$ for the cubes and $V = HL^2$ for the film geometry. We have calculated the specific heat using the expression

$$c = VT^{-2} (\langle e^2 \rangle - \langle e \rangle^2). \tag{4}$$

The above thermal averages denoted by the angular brackets are computed according to

$$\langle O \rangle = Z^{-1} \int \prod_i d\theta_i O[\theta] \exp(-\beta \mathcal{H}), \tag{5}$$

where $\mathcal{H} = H/J$ is the energy in units of J and $\beta = J/T$. Here $O[\theta]$ denotes the dependence of the physical observable O on the configuration $\{\theta_i\}$, and the partition function Z is given by

$$Z = \int \prod_i d\theta_i \exp(-\beta \mathcal{H}). \tag{6}$$

We computed the specific heat $c(T,L)$ of the x-y model as a function of temperature on several cubic lattices L^3 (with $L = 20,30,40,50$). Open (free) boundary conditions were applied in all directions; namely, the spins on the surface of the cube are free to take any value. These spins interact only with the five nearest neighbors, one in the interior and four on the surface of the cube, and there is one missing neighbor. We have also calculated the specific-heat scaling function $f_1(x)$ (to be defined in the following section) for the case of the parallel-plate geometry $L_1 \times L_2 \times L$ $(L_{1,2} \gg L)$ using periodic boundary conditions along the long directions of the film and open BC's along the thickness direction L. For this case we need to take the limit $L_{1,2} \to \infty$ first; in Ref. 10 , it was found that using $L_1 = L_2 = 5L$ was large enough, in the sense that systematic errors due to the finite-size effects from the fact that $L_{1,2}$ are not infinite are smaller than the statistical errors for realistic computational time scales. The present simulations for films were done on lattices $60 \times 60 \times 12$, $70 \times 70 \times 14$, and $80 \times 80 \times 16$. Calculation for such films with Dirichlet BC's (which are achieved using an antiferromagnetic pseudospin alignment for the spins on the boundary) were reported in Refs. 9 and 10.

We used the Monte Carlo (MC) method and in particular Wolff's cluster algorithm.[15] We carried out of the order of 30 000 MC steps for thermalization to obtain equilibrium configurations. We made of the order of 10 000–50 000 measurements allowing 500 MC steps between successive measurements to obtain statistically uncorrelated configurations.

III. SCALING FUNCTIONS

The main goal of this paper is to present a calculation of the specific-heat scaling function for the case of cubic confinement and open BC's. In this calculation we have used open BC's in all three directions of the cube. We found that using open BC's the results for the specific-heat scaling were very close to those obtained with Dirichlet BC's. This will be demonstrated in the next section where we compare the previously published results[9,10] for films with Dirichlet BC's and results reported in this paper for films with open BC's.

One can imagine a number of different scaling functions for the specific heat. Any dimensionless combination such as the ratio given by Eq. (1) can be used as a scaling function. However, the various experimental groups have extracted two scaling functions, the so-called $f_1(x)$ and $f_2(x)$ with $x = tL^{1/\nu}$. These scaling functions are defined as follows:

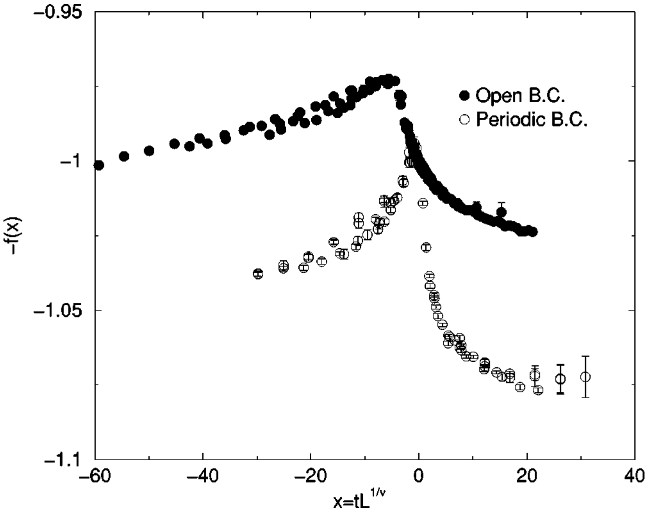

FIG. 1. The scaling function $-f(x)$ defined by Eq. (1).

$$c(t,L)-c(t_0,\infty)=L^{\alpha/\nu}f_1(tL^{1/\nu}), \tag{7}$$

$$[c(t,\infty)-c(t,L)]t^{\alpha}=f_2(tL^{1/\nu}). \tag{8}$$

We limit our goal to calculate the specific-heat scaling function for the confined geometry and not the bulk critical exponents or critical amplitude ratios. We take the values for the bulk critical exponents and the universal amplitude ratios as determined experimentally.[17] Previous MC work such as the work of Ref. 16 shows that the critical exponents are within error bars from the experimental values. Recent analysis of the most accurate experimental results for bulk helium[17] finds good agreement with the theoretical results[18] for the critical exponents. Our approach to use the experimentally determined values of the critical exponents and amplitude ratios and to determine the scaling function by applying FSS on the calculated $c(t,L)$ has no fitting parameters and this allows no ambiguity. Therefore we use $\nu=0.6709$ as obtained from accurate experiments[17] such as the so-called lambda point experiment (LPE), an experiment in microgravity environment. The hyperscaling relation $\alpha=2-3\nu$ yields $\alpha/\nu=-0.0189$, and the correlation length $\xi(t)=\xi_0^{\pm}|t|^{-\nu}$ becomes equal to the system size L at the reduced temperature t_0, i.e., $t_0=(\xi_0^+/L)^{1/\nu}$ with $\xi_0^+=0.498$.

In order to find the universal function $f(x)$ defined by Eq. (1), we need to know $c(0,\infty)$. We use the bulk values for $c(0,\infty)$ obtained by studying the finite-size scaling of the specific heat of cubes with periodic BC's.[16] In Fig. 1 the scaling function $-f(x)$ obtained for cubes with open BC's in all three directions is compared to that obtained with periodic BC's.[16]

The scaling function $f_1(x)$ [Eq. (7)] can be calculated using our calculated $c(t,L)$ and

$$c(t_0,\infty)=c(0,\infty)+c_1^+t_0^{-\alpha}, \tag{9}$$

where the values of $c(0,\infty)$ and c_1^+ for the x-y model are obtained from Ref. 16.

In order to calculate the universal function $f_2(x)$ [Eq. (8)], we need to know the bulk specific heat $c(t,\infty)$ also. Since we are restricting ourselves to the critical region, we may write the following:

$$c(t>0,\infty)=c(0,\infty)+c_1^+t^{-\alpha}, \tag{10}$$

$$c(t<0,\infty)=c(0,\infty)+c_1^+/r|t|^{-\alpha}, \tag{11}$$

$$r=\frac{c_1^+}{c_1^-}, \tag{12}$$

where r is the universal amplitude ratio and it is most accurately determined experimentally[17,19] from the critical properties of bulk helium to be $r=1.053(2)$ (Ref. 17). Inserting Eqs. (10) and (11) into Eq. (8), we obtain

$$f_2(tL^{1/\nu})=[c(0,\infty)-c(t,L)]t^{\alpha}+c_1^+, \quad t>0, \tag{13}$$

$$f_2(tL^{1/\nu})=[c(0,\infty)-c(t,L)]|t|^{\alpha}+c_1^+/r \quad t<0, \tag{14}$$

which can be calculated by using our computed $c(t,L)$ and the values of $c(0,\infty)$ and c_1^+ from Ref. 16.

IV. FILMS WITH OPEN BOUNDARY CONDITIONS

In Refs. 9 and 10 the specific-heat scaling function for a parallel-plate geometry on lattices of size $L_1\times L_2\times L$ with $L_1=L_2\gg L$ was calculated. In Refs. 9 and 10 periodic BC's along the $L_{1,2}$ directions and staggered (Dirichlet) BC's or periodic BC's along the film-thickness direction of size L were applied. It was found that while the calculated scaling function for the parallel-plate geometry using periodic BC's along all three directions was very different from that obtained with Dirichlet BC's along the top and bottom of the plate and periodic BC's along the other two long directions, the latter scaling function fits the experimental results with no free parameter. This was explained on the basis that physically the order parameter along the film thickness vanishes at the boundaries of the film and therefore Dirichlet BC's are more appropriate.

In this paper we have used open BC's along the top and bottom of the plate, instead of Dirichlet BC's, and periodic BC's along the two long directions of the plate. Since the film terminates on the top and bottom surfaces, for the pseudospins which belong to these two surfaces (in the language of the x-y model) there are no neighboring spins beyond the top and bottom surface planes of the plate. Therefore, even if we use open (free) boundary conditions, this termination acts as a "zero-order parameter constraint" beyond the top and bottom of the plate. This implies that these two BC's—namely, staggered BC's and open BC's—are very similar for thick enough films.

In order to make a direct comparison of our calculated $f_1(x)$ to the experimental $f_1(x)$, we express all lattice units in physical units using the following equation:[9]

$$f_1(x)|_{phys}=\lambda f_1(x)|_{lattice}, \tag{15}$$

$$\lambda\equiv\frac{V_m k_B}{a^3}(a/\text{Å})^{-\alpha/\nu}, \tag{16}$$

where V_m is the molar volume of liquid helium at the λ point and saturated vapor pressure, k_B is Boltzmann's constant, and a the lattice spacing in the x-y model required to make

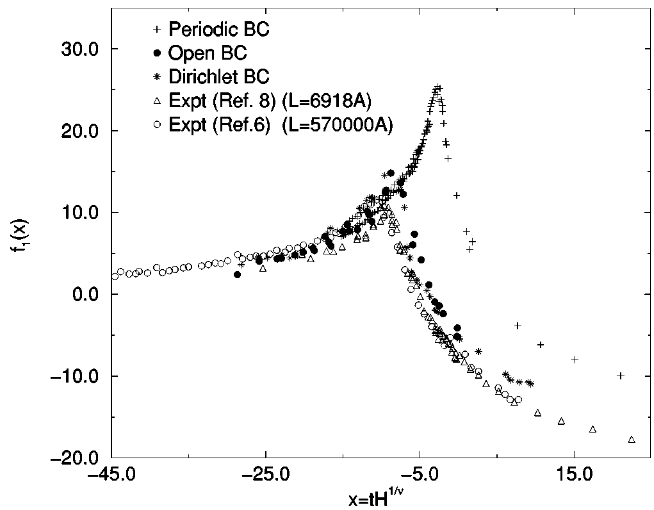

FIG. 2. Film geometry: the computed universal function $f_1(x)$ with open BC's (solid circles) is compared to the previously calculated scaling function using Dirichlet BC's (Ref. 9) (data shown as stars) and periodic BC's (shown as plus signs) and the experimental results of Lipa *et al.* (Ref. 6) (open circles) and those of Mehta *et al.* (Ref. 8) (open triangles).

contact with the critical behavior of the correlation length in helium. This prefactor $\lambda = 15.02$ J/(K mol) and it was determined in Ref. 9.

In Fig. 2 we compare the results for f_1 for the case of films obtained with open BC's along the direction of the film thickness to those obtained earlier[9,10] and to the experimental results.[6,8] It is clear that within error bars our results for the specific-heat scaling function are the same for both cases of BC's.

While the scaling function is sensitive to boundary conditions, this indicates that it is hard to distinguish Dirichlet from open BC's for the specific-heat scaling function. We feel that when we use physical BC's the agreement between the theoretical results for the specific-heat scaling function and the experimental results is quite good taking into consideration the fact that there is no free parameter.

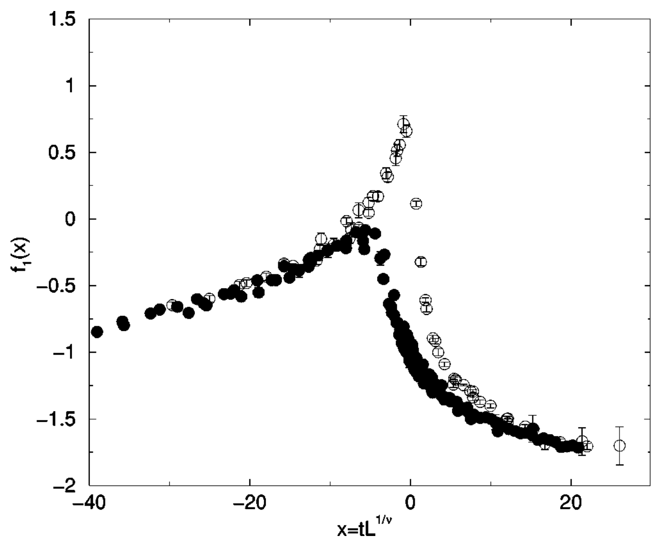

FIG. 3. The scaling function $f_1(x)$ obtained for cubes of size L^3 with open (solid circles) and that obtained for cubes with periodic BC's (open circles) are compared.

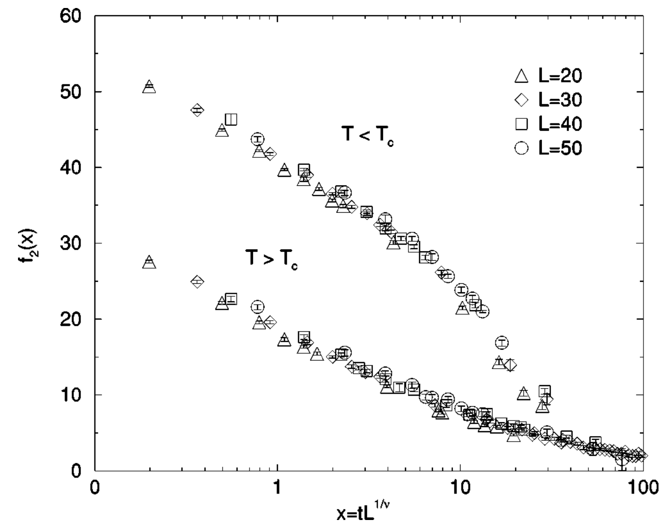

FIG. 4. The universal function $f_2(x)$ for cubes of size L^3 with open boundary conditions.

V. CUBIC CONFINEMENT

In this section we present the results for the scaling functions $f_1(x)$ and $f_2(x)$ obtained for cubes of size L^3 with $L = 20,30,40,50$ using open and periodic BC's in all three directions. As was shown in the previous section open (free) BC's are similar to using Dirichlet BC's and they both express the physical condition imposed by the confinement or the termination of the system. In Fig. 3 we compare the scaling function $f_1(x)$ obtained for open BC's with that obtained for periodic BC's.[16] Notice the suppression of $f_1(x)$ when calculated with open BC's relative to the case of periodic BC's. This is similar to the case of the parallel-plate geometry (Fig. 2). The scaling functions $f_1(x)$, however, are

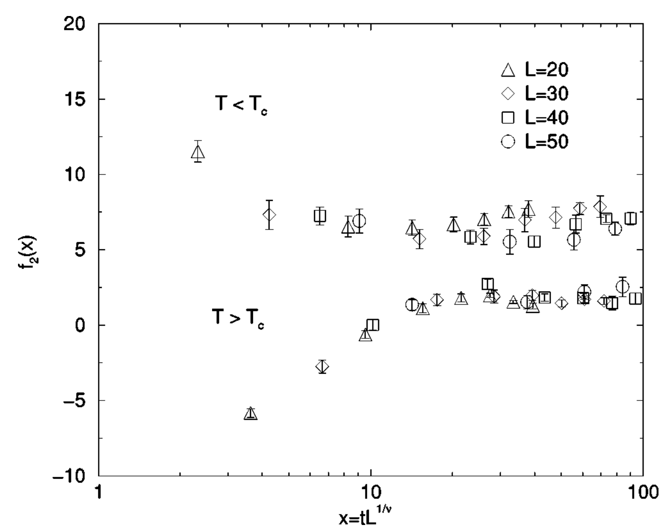

FIG. 5. The universal function $f_2(x)$ for cubes of size L^3 with periodic boundary conditions.

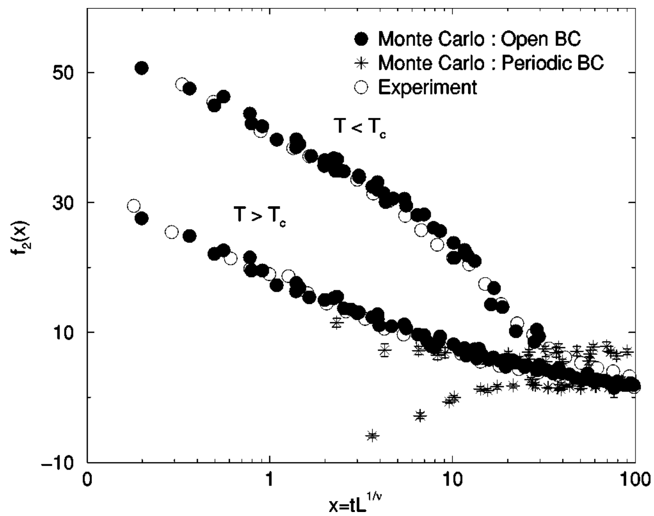

FIG. 6. The computed universal function $f_2(x)$ for open and periodic BC's and for cubes is compared to the experimental results (Refs. 13 and 14).

very different for cubic and parallel-plate geometry. Notice, for instance, that for the case of cubic confinement with open BC's $f_1(x)$ is negative for all values of x, something very different from what happens for any of the calculated or the experimental scaling functions for parallel-plate confinement.

In Fig. 4 we give the results of our present Monte Carlo calculation of the function $f_2(x)$ for cubes with open BC's using Eqs. (13) and (14). Figure 5 shows the results of our calculation with periodic boundary conditions. Figure 6 compares the scaling function $f_2(x)$ obtained for open BC's and for periodic BC's. Notice the qualitatively different behavior for the same scaling function for the same geometry but different boundary conditions.

Experimentally the universal scaling function $f_2(x)$ for cubic confinement has just become available.[13,14] In order to make a direct comparison of our calculated scaling function $f_2(x)$ to the experimentally determined, we express all lattice units in physical units. The prefactor is the same as in the case of the function $f_1(x)$:

$$f_2(x)|_{phys} = \lambda f_2(x)|_{lattice}, \tag{17}$$

where λ is the constant given in the previous section by Eq. (16) and its numerical value is $\lambda = 15.02$ J/(K mol).

In Fig. 6, $f_2(x)$ obtained from our MC calculation is compared with the experimental data.[13,14] The agreement between the scaling function calculated with open BC's and experiment is quite satisfactory considering the fact that there is no free parameters.

VI. CONCLUSIONS

In this paper we have used the x-y model which describes the fluctuations of the superfluid order parameter near the critical point to calculate the scaling functions associated with the specific heat for the case where the superfluid is confined in a cubic geometry and in parallel-plate geometry. Both in the theoretical calculations and in the experiments, the region very near the superfluid transition is probed such that the correlation length associated with the superfluid order parameter is of the size of the confining length.

First, we calculated the specific-heat scaling function for the case of parallel-plate confining geometry using open boundary conditions along the top and bottom surfaces of the film. Our results are very close to those obtained[9,10] with Dirichlet (staggered BC's) along the top and bottom surfaces of the film. Both calculations are in satisfactory agreement with experimental results[6–8] while the results of earlier calculations using periodic boundary conditions[16] were found to disagree with the experimental scaling function near the superfluid transition.

Just recently, experimental measurements[13,14] on superfluid helium confined in cubes became available. This prompted us to calculate the heat-capacity scaling function of superfluids for cubic confinement. When we used open boundary conditions in all three directions of the cube we find very good agreement between the calculated and the measured[13,14] scaling functions with no adjustable parameter. On the contrary, if periodic boundary conditions are used at the boundaries of the cube, which are unphysical boundary conditions for a confined system, there is great disagreement between the calculated and measured specific-heat scaling functions.

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