Rapid Communication

Scaling of the superfluid density in superfluid films

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We study scaling of the superfluid density with respect to the film thickness by simulating the $x - y$ model on films of size $L \times L \times H$ ($L >> H$) using the cluster Monte Carlo. While periodic boundary conditions where used in the planar (L) directions, Dirichlet boundary conditions where used along the film thickness. We find that our results can be scaled on a universal curve by introducing an effective thickness. In the limit of large H our scaling relations reduce to the conventional scaling forms. Using the same idea we find scaling in the experimental results using the same value of $\nu = 0.6705$.
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Scaling is a central idea in critical phenomena near a second order phase transition and in field theory when we are interested in the continuum limit.[1] In both cases we are looking at the singular behavior emerging from the overwhelmingly large number of degrees of freedom, corresponding to the original cutoff scale, which need to be integrated out leaving behind long-wavelength degrees of freedom which vary smoothly. Their behavior is controlled by a dynamically generated length scale, the correlation length ξ. Such a fundamental idea is difficult to test theoretically because it requires a study of an overwhelmingly large number of interacting degrees of freedom. Experimentally, however, one hopes to be able to study scaling in finite-size real systems near a second order phase transition. Namely, the system is confined in a finite geometry (for example, film geometry) and the finite-size scaling theory is expected to describe the behavior of the system near the

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bulk critical temperature T_λ. Liquid ^4He has been a good real system for testing finite-size scaling theory and measuring the critical exponents that are associated with the most singular behavior in thermodynamic quantities near T_λ. However, measurements of the superfluid density[2] of helium films failed to verify the finite-size scaling theory. A recent reanalysis[4] of the specific heat data reported in Refs. 3 and also new measurements of the specific heat[5] show good agreement with finite–size scaling theory for the specific heat. It has also become clear that the choice of the boundary conditions[4,6,7] is a key factor in comparing the more recent measurements of the universal function[5] and that obtained theoretically. On the other hand, while new experiments for the specific heat under confined geometries have been planned to be conducted under more ideal microgravity conditions,[8] the problems related to the measurements of the superfluid density[2] are still outstanding. (For a comprehensive review of experiments on ^{4}He to test the finite–size scaling theory cf. Ref. 9.)

In this paper we use the $x-y$ model and the cluster Monte Carlo method to calculate the *superfluid density* on films of size $L \times L \times H$ $(L >> H)$ with periodic boundary conditions in the planar L-directions and Dirichlet boundary conditions (vanishing order parameter) along the film thickness dimension. The same model, geometry, and boundary conditions where used in Ref. 6 to calculate the *specific heat*, and a reasonable agreement between the theoretically calculated and experimentally determined universal functions was found. In this paper we show that the superfluid density is a far more sensitive observable than the specific heat with respect to the requirement that one needs to use very thick films $(H \to \infty)$ to verify scaling with respect to the film thickness H. We have found that in order to achieve scaling for rather small values of H (as in the case of the specific heat) we need to modify the scaling expressions by using a concept of an effective thickness. Our introduction of an effective thickness $H_{eff} = H + D$ (where D is a finite dynamically generated length scale) is no violation of scaling, since at large H_{eff} the constant D can be neglected. Scaling for all the values of H used in our calculation is achieved with the expected value of $\nu = 0.6705$.[10] A similar modification to the scaling formula allows scaling of the experimental results of Rhee et al.[2] for the superfluid density with the same value of ν.

For the $x-y$ model on a lattice, the helicity modulus $\Upsilon_\mu(T)/J$ as defined in Refs. 11 is calculated as the ensemble average of $1/V(\sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)(\vec{e}_\mu \cdot \vec{\epsilon}_{ij})^2 - \beta(\sum_{\langle i,j \rangle} \sin(\theta_i - \theta_j)\vec{e}_\mu \cdot \vec{\epsilon}_{ij})^2)$. Here V is the volume of the lattice, $\beta = J/k_BT$, $\vec{e}_\mu$ is the unit vector in the corresponding bond direction, and $\vec{\epsilon}_{ij}$ is the vector connecting the lattice sites i and j. In the following we omit the vector index since we will always refer to the x-component of the

helicity modulus and due to the isotropy $\Upsilon_x = \Upsilon_y$. The connection between the helicity modulus and the superfluid density ρ_s is established by the relation[12] $\rho_s(T) = (m/\hbar)^2 \Upsilon(T)$ where m denotes the mass of the helium atom.

In Ref. 13 we studied the helicity modulus Υ for the $x - y$ model in a film geometry with *periodic* boundary conditions in the H-direction. In a certain temperature range around the bulk critical temperature T_λ where the bulk correlation length $\xi(T)$ becomes of the order of the film thickness H the quantity $\Upsilon H/T$ exhibits effectively two–dimensional behavior and a Kosterlitz–Thouless phase transition takes place at a temperature $T_c^{2D}(H) < T_\lambda$. We found that the critical temperature $T_c^{2D}(H)$ approaches T_λ in the limit $H \to \infty$ as

$$T_c^{2D}(H) = T_\lambda \left(1 + \frac{x_c}{H^{1/\nu}} \right), \tag{1}$$

where the critical exponent ν is the same as the experimental value $\nu = 0.6705$[10] and the value $T_\lambda/J = 2.2017$.[14] We also demonstrated that $\Upsilon H/T$ is a function of the ratio $H/\xi(T)$, i.e. the dimensionless quantity

$$\frac{\Upsilon(T,H)H}{T} = \Phi(tH^{1/\nu}), \tag{2}$$

is a function of $x = tH^{1/\nu}$ only. We found that when we plotted the calculated $\Upsilon(T,H)H/T$ as a function of x, in the limit $L \to \infty$, our results for all thicknesses H collapse onto the same universal curve. Thus, simple scaling holds for periodic boundary conditions.

In this paper we consider periodic boundary conditions in the planar L-directions and Dirichlet boundary conditions (represented by a staggered spin configuration in the boundary layer) along the thickness direction. Fig. 1 displays our Monte Carlo data for the helicity modulus in units of the lattice spacing a and the energy scale J for the film of fixed thickness $H = 4$. Dirichlet boundary conditions strongly suppress the values of the helicity modulus as compared to the case of periodic boundary conditions along H. As a consequence, films with Dirichlet boundary conditions have lower critical temperatures than films with periodic boundary conditions.

We eliminate the finite size effects in the L-direction by studying the quantity $K = T/(\Upsilon H)$ in the $L \to \infty$ limit. For a fixed thickness H and at temperatures T below but sufficiently close to the critical temperature $T_c^{2D}(H)$, the system behaves effectively two–dimensionally.[13,15] It was demonstrated in Ref. 13 that we can use the Kosterlitz–Thouless–Nelson renormalization group equations[16] to derive an expression for the planar L-dependence of K. This expression can be used to extrapolate the computed values $K(T,H,L)$ obtained on lattices of finite L to the $L = \infty$ limit, for
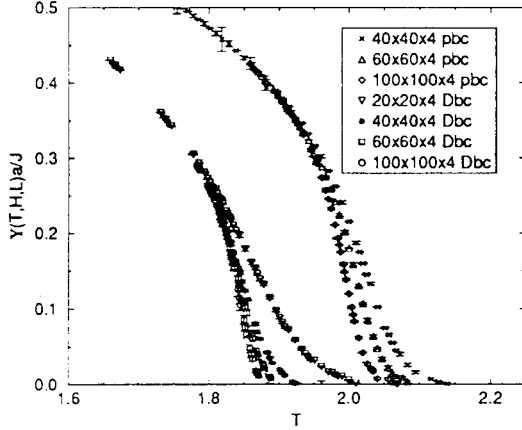
Fig. 1. The helicity modulus $\Upsilon(T, H, L)$ as a function of T for various lattices $L^2 \times 4$ with Dirichlet boundary conditions (Dbc) in the H-direction.

a fixed H. This has been clearly demonstrated in Ref. 13 for the case of periodic boundary conditions. The quality of our extrapolation is the same as in Ref. 13 and we omit such demonstration here due to lack of space. In the following we shall drop the dependence of Υ on L implying that we refer to the extrapolated $L \rightarrow \infty$ values.

In Fig. 2 we plot $\Upsilon(T, H)H/T$ versus $tH^{1/\nu}$ for the thicknesses $H = 12, 16, 20, 24$ to check the validity of the scaling form (2) using the experimental value of $\nu = 0.6705$.[10] We do not obtain a universal scaling curve, thus scaling according to the expression (2) is not valid for the films with thicknesses up to $H = 24$.

Let us, therefore, pursue another line of thought. In Fig. 3 we show the layered helicity modulus $\Upsilon_L(z)/J$, where z counts the layers, computed on a $60 \times 60 \times 20$ lattice at the temperature $T/J = 2.1331$. The quantity $\Upsilon_L(z)/J$ is just the helicity modulus determined for each layer separately. The layered helicity modulus is symmetric with respect to the middle layer where it reaches its maximum and decreases when the boundaries are approached. Although the helicity modulus $\Upsilon(T, H, L)/J$ is not the average of the quantity $\Upsilon_L(z)/J$ over all layers, the curve in Fig. 3 is an approximation to the profile that the superfluid density develops in thin films. The basis for the standard scaling argument is the following. For large H and very close to the critical point where $\xi(T)$ is very large, the "penetration" depth $\lambda(T)$ of the superfluid density inside the film is of the order of the correlation length.
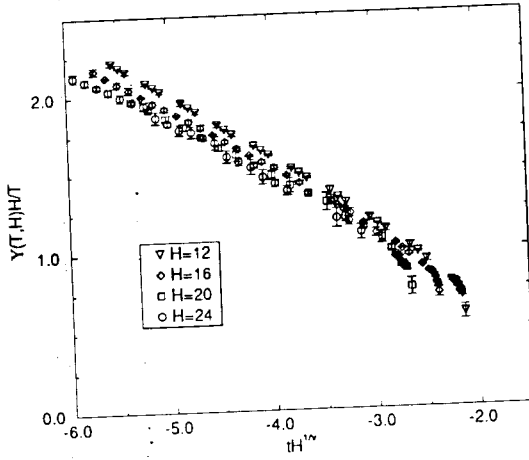
Fig. 2. $\Upsilon(T, H)H/T$ as a function of $tH^{1/\nu}$ for various thicknesses. $\nu = 0.6705$.
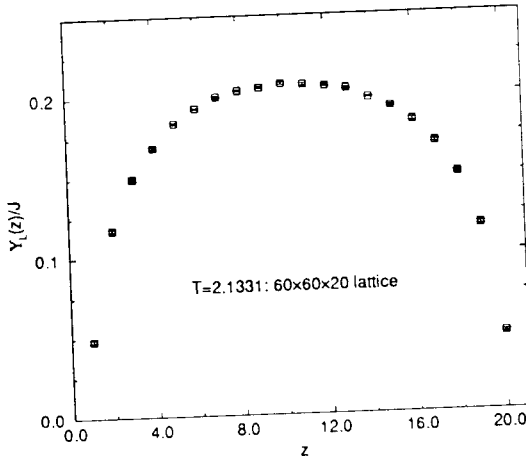

Fig. 3. The approximate profile $\Upsilon_L(z)$ of the helicity modulus computed on a $60 \times 60 \times 20$ lattice at $T = 2.1331$, i.e. close to the critical temperature, $T_c^{2D}(20) = 2.1346$.

Thus, in the limit where all other length scales are small compared to H and ξ, if we plot YH versus z/H (or z/ξ) we should find scaling. However, for small H there is at least one length scale D (which for $H \sim D$ needs to taken into account) which has the following origin. The length scale D contains information on how fast $\Upsilon(z)$ rises from $\Upsilon(z = 0) = 0$. Namely the z-derivative of $\Upsilon(z)$ is not universal, it depends on how we have imposed the Dirichlet boundary conditions. There are many ways to make the order parameter vanish at the boundary. It can be made to be zero when averaged over a boundary area $A = l \times l$. In our case of staggered boundary conditions $l = \sqrt{2}$. If we had chosen Dirichlet boundary conditions where the order pa-rameter is zero over an area with $l > \sqrt{2}$ we would have found a slower rise of $\Upsilon(z)$ from its zero value at the boundary. If this initial "faster rise" of the superfluid density is neglected, the rest of $\Upsilon(z)$ can be fit to $A \cosh(z/\xi) + B$ with only one length scale, the correlation length ξ. Thus the curve $Y(z)$ can be thought of as made of two contributions, and scaling at small values of H can be obtained only if the film size is extended. We can imagine that this thinner film of size H is obtained from a thicker one by a process of forcing the superfluid density to go to zero faster than its "natural way" by a "speed" dictated by the severity of the boundary conditions.
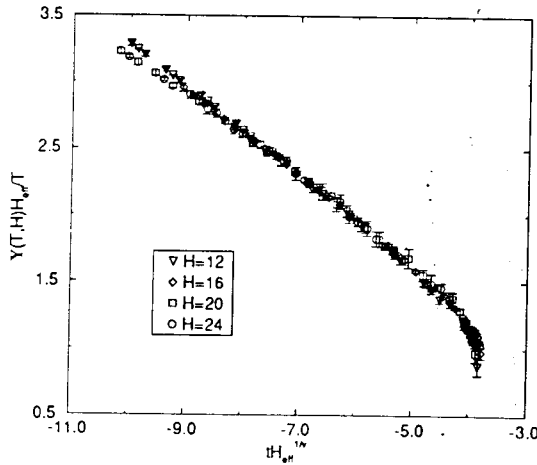

Fig. 4. $\Upsilon(T, H)H_{eff}/T$ as a function of $tH_{eff}^{1/\nu}$ for various thicknesses. $H_{eff} = H + 5.79$ and $\nu = 0.6705$.

The lack of scaling with the expected critical exponent $\nu = 0.6705$ indicates that the critical temperatures $T_c^{2D}(H)$ do not satisfy Eq. (1).

Because of the argument given earlier about the profile of the superfluid density we may expect an effective film thickness H_{eff} to enter the scaling expressions (1) and (2). The simplest assumption is $H_{eff} = H + D$ where D is a constant. Indeed by replacing H with H_{eff} in these equations for the film thicknesses $H = 12, 16, 20$ we obtain $x_c = -3.81(14)$ and $D = 5.79(50)$ with $\nu = 0.6705$. In Fig. 4 we plot $\Upsilon(T, H)H_{eff}/T$ as a function of $tH_{eff}^{1/\nu}$ for films with $H = 12, 16, 20, 24$ where $\nu = 0.6705$. The data for the helicity modulus collapse approximately onto one universal curve.
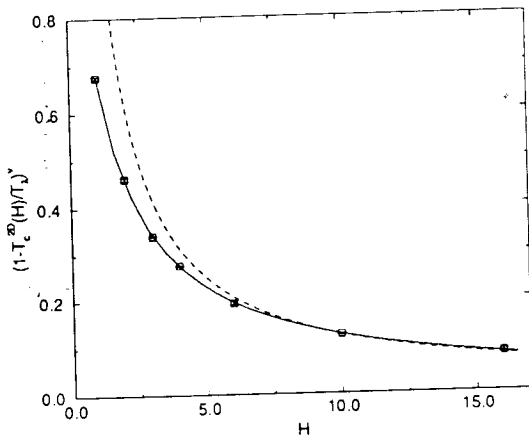

Fig. 5. $(1 - T_c^{2D}(H)/T_\lambda)^\nu$ for the Villain model in a film geometry with open boundary conditions as a function of H. The solid line is the expression $1.62^\nu/(H + 1.05)$, $\nu = 0.6705$. The dashed line represents the expression $1.25/H$ (fit to the last two data points).

We wish to test further the assumption that the boundaries introduce an effective thickness into the scaling expression (2). Janke and Nather[17] studied the thickness dependence of the Kosterlitz–Thouless transition temperature of the Villain model with open boundary conditions (interactions of the top and bottom layer only with the interior film layers). They found, however, that in order for scaling to occur they needed to use a value for ν higher than the value believed for the model. We replace H in Eq. (1) by the effective thickness $H_{eff} = H + D_V$. Indeed, taking the expected value $\nu = 0.6705$ we find $D_V = 1.05(2)$ and $x_c = -1.62(2)$ and a good quality of fit (cf. Fig. 5). In Fig. 5 we also included the result of the fit of the Kosterlitz–Thouless transition temperatures $T_c^{2D}(H)$ to the expression (1) where we fixed the value of the critical exponent ν at the expected value

0.6705 (dashed line). Only when the transition temperatures corresponding to the thicknesses $H = 10$ and $H = 16$ were used for the fit we obtained a good quality of the fit.

We can understand the increment D as an effective scaling correction which renders the scaling relations (1) and (2) valid even for very thin films. This scaling correction is of zeroth order in the reduced temperature and can thus be assumed to be a constant. Furthermore, since the increment D is due to excessive vortex creation by the boundaries and scaling is only valid in a narrow temperature region about T_λ, we may assume the vortex creation rate, and thus the increment D, to be only weakly temperature dependent. For large thicknesses H the increment D can be neglected and we recover the conventional scaling forms. This result means that the film thicknesses considered in Ref. 17 were still too small to extract the expected value of the critical exponent ν from the H–dependence of the critical temperature (1) without the help of an effective thickness $H + D_V$.
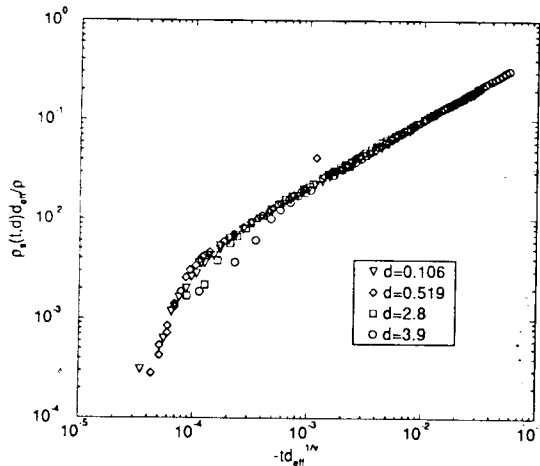

Fig. 6. Scaling of the superfluid density data of Rhee et al.[2] with the effective thickness $d_{eff} = d + 0.145$. $\nu = 0.6705$ and all lengths are in μm.

In the experimental situation it is possible to imagine a similar situation where a length scale D emerges and corresponds to an average distance on the substrate over which vortices are created. (In the experiments by Rhee et al.[2] the supporting pillars could be a source for additional vortex creation.) In Fig. 6 we achieve approximate collapse of the data for the superfluid density ρ_s for films of various thickness d (d is in μm) given in Refs. 2 by

plotting $\rho_s(t,d)d_{eff}/\rho$ versus $td_{eff}^{1/\nu}$ with $\nu = 0.6705$ and $d_{eff} = d + 0.145$. We obtained the effective thickness by examining the reduced temperatures $t_{fs}(H)$ where finite–size effects set in. According to finite–size scaling theory t_{fs} has to fulfill the relation $t_{fs} \propto d^{-1/\nu}$, thus in our case $t_{fs} \propto d_{eff}^{-1/\nu}$. The data points corresponding to the film with $d = 3.9\mu m$ deviate from the universal curve; we attribute this to the anomalous behavior of these data. Namely, in general $|t_{fs}(d_1)| > |t_{fs}(d_2)|$ if $d_1 < d_2$, but this is not the case for $d_1 = 2.8\mu m$ and $d_2 = 3.9\mu m$ (cf. Refs. 2). The scaling of the experimental data with the aid of this finite length scale indicate that the average distance between defects will introduce a new length scale from which has to be much smaller than the film thickness and the correlation length to see simple finite size scaling. Theoretically there are two different limits in which simple scaling with H should be expected to be valid. The clean boundary limit, $\xi \sim H \ll D$, and the dirty boundary limit where $D \ll \xi \sim H$.

In conclusion, we find that the results of our simulations for the super-fluid density on rather small thickness films obey a scaling relation where an effective thickness is introduced. Conventional scaling relations is expected to be valid on films of much larger thickness. Applying the same idea of the effective thickness on the experimental data, we found that we were able to scale the data of Rhee et al.[2] in a simple way without resorting to any departure from scaling nor to using unrealistic values for ν. Clearly, more experiments with different substrates are desirable.

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