Possible Resolution of the Finite-Size Scaling Problem in ^{4}He

W. Huhn and V. Dohm

Insitut für Theoretische Physik, Technische Hochschule Aachen, D-5100 Aachen, West Germany

(Received 28 January 1988)

We offer an explanation of the long-standing discrepancy between finite-size scaling theory and the observed temperature shift $T_\lambda - T_m$ of the specific-heat maximum in confined ^{4}He. On the basis of a renormalization-group calculation using Dirichlet boundary conditions we argue that a new size-dependent scaling variable should be employed. The theory agrees with the data in the regime $T_\lambda \gtrsim T_m$ without an adjustment of parameters and explains the gradual onset of finite-size effects far from T_λ.

PACS numbers: 67.40.Kh, 05.70.Jk, 64.60.Fr

Since the early formulation of a phenomenological finite-size scaling theory of critical phenomena[1] there have been numerous theoretical studies and computer simulations on this subject.[2] Among the very few attempts to verify this theory by experiments *in real systems* there exists only one set of data at the required level of accuracy: the measurements of the critical specific heat and superfluid density in confined ^{4}He by Gasparini and co-workers.[3,4] It has therefore been a severe disappointment that just these data appear to contradict the scaling theory.

The purpose of this Letter is to present detailed arguments and quantitative results that point towards a natural explanation of this long-standing problem. Our reasoning will be based entirely on the conventional Landau-Ginzburg-Wilson Hamiltonian for the n-component order parameter $\phi(x)$ ($n=2$ for ^{4}He),

$$H_\phi = \int d^dx [\tfrac{1}{2} r_0\phi^2 + \tfrac{1}{2}(\nabla\phi)^2 + u_0\phi^4], \tag{1}$$

without accepting unusually large[5] correction-to-scaling amplitudes or invoking[6] surface fractal dimensionalities. Our new point is to incorporate fairly realistic (Dirichlet) boundary conditions (vanishing order parameter at the walls) in a quantitative renormalization-group calculation. No adjustment of nonuniversal amplitudes or couplings will be necessary because they are known from bulk theory[7] and independent bulk data.[8]

Specifically, we shall discuss the heat capacity C of ^{4}He confined in a geometry of size L. Our attention will be focused not only on the temperature shift[3] $T_\lambda - T_m(L)$ of the specific-heat maximum and on the rounding temperature[1,2] $T^*(L)$, but also on a detailed comparison of the predicted T and L dependence of $C(T,L)$ with the data in the regime $T \gtrsim T_m$. We shall show that Dirichlet boundary conditions (Dbc) have an unexpectedly large effect on these quantities. In particular, the conventional power law,[1,2]

$$T_\lambda - T_m(L) \sim L^{-1/\nu}, \tag{2}$$

where the bulk-correlation-length exponent is $\nu \simeq 0.67$, and should be replaced by

$$T_c(L) - T_m(L) \sim L^{-1/\nu}, \tag{3}$$

where $T_c(L) < T_\lambda$ is an *intrinsic reference temperature*, the introduction of which suggests itself in the analysis. Furthermore, we find a gradual onset of finite-size effects far from T_λ, which explains why previous results[3] concerning $T^*(L)$ were inconclusive.

In order to substantiate these points it is necessary to describe our calculation in some detail. We have generalized the approach of Refs. 9 and 10 to the case of a cube with Dbc in $\tilde d$ directions and periodic boundary conditions (pbc) in $d-\tilde d$ directions. For simplicity we first consider $\tilde d = d$ and $n=1$. This case has been discussed recently[11] for $d>4$ where the bulk critical behavior is mean-field-like. Here we shall study the relevant case $d<4$. We expand $\phi(x)$ in standing-wave modes,

$$\phi(x) = 2^{d/2}\left[\phi_1 \prod_{j=1}^{d} \sin(\pi x_j/L) + L^{-d/2} \sum_n{}' \phi_{\mathbf n} \prod_{j=1}^{d} \sin(\pi n_j x_j/L)\right], \tag{4}$$

with $\mathbf{n} \equiv (n_1, \ldots, n_d)$, where $\sum'$ denotes the sum over all modes (positive integers n_j) except for the lowest mode $\sim\phi_1$ (all $n_j = 1$). Accordingly, we split $H_\phi = H_1 + H(\phi_{\mathbf n})$, where

$$H_1(\phi_1) = L^d[\tfrac{1}{2}(r_0 + \tilde d\pi^2/L^2)\phi_1^2 + \tilde u_0 \phi_1^4] \tag{5}$$

with $\tilde u_0 = (\tfrac{3}{2})^{\tilde d} u_0$, and

$$H(\phi_{\mathbf n}) = \tfrac{1}{2} \sum_{\mathbf{n},\mathbf{n}}{}' \phi_{\mathbf n} A(\mathbf{n},\mathbf{n}') \phi_{\mathbf n'} + w_0 \sum_n{}' \phi_{\mathbf n} \prod_{j=1}^{d} \Delta(n_j) \tag{6}$$

with $w_0=4L^{d/2}\tilde{u}_0\phi_{\mathbf{1}}^3$ and $\Delta(n_j)\equiv\delta_{1n_j}-\frac{1}{3}\delta_{3n_j}$. In Eq. (6) we have neglected terms of $O(\phi_{\mathbf{n}}^3,\phi_{\mathbf{n}}^4)$ as is appropriate within a one-loop approximation. The matrix elements $A(\mathbf{n},\mathbf{n}')$ read

$$A(\mathbf{n},\mathbf{n}')=(r_0+\pi^2\mathbf{n}^2/L^2)\prod_{j=1}^{d}\delta_{n_jn_j'}+6u_0\phi_{\mathbf{1}}^2\prod_{j=1}^{d}(2\delta_{n_jn_j'}+\delta_{2,n_j+n_j'}-\delta_{n_j-2,n_j'}-\delta_{n_j+2,n_j'}). \tag{7}$$

Integration over $\phi_{\mathbf{n}}$ yields the partition function $Z=\int d\phi_1\exp(-H_1-\Gamma)$ with

$$\Gamma=\tfrac{1}{2}\,\mathrm{Tr}\ln A-\tfrac{1}{2}w_0^2\sum_{\mathbf{n},\mathbf{n}'}{}'\prod_{j=1}^{d}\Delta(n_j)A^{-1}(\mathbf{n},\mathbf{n}')\Delta(n_j'). \tag{8}$$

The final step consists in an expansion of $\Gamma(\phi_{\mathbf{1}}^2)$ around

$$\langle\phi_{\mathbf{1}}^2\rangle_1=Z_1^{-1}\int d\phi_1\,\phi_{\mathbf{1}}^2\exp(-H_1)\equiv M. \tag{9}$$

The explicit calculation, e.g., of the specific heat $C_\phi=4L^{-d}\partial^2\ln Z/\partial r_0^2$ is considerably more complicated than in the case of pbc since A is nondiagonal. The most significant difference shows up in typical sums such as

$$S_{\mathrm{Dbc}}(\hat{r}_0,L)=L^{-d}\sum_{\mathbf{n}}{}'(\hat{r}_0+\pi^2\mathbf{n}^2/L^2)^{-2} \tag{10}$$

with $\hat{r}_0=r_0+12\tilde{u}_0M$. The corresponding sum in the case of pbc reads

$$S_{\mathrm{pbc}}(\bar{r}_0,L)=L^{-d}\sum_{\mathbf{n}}{}'(\bar{r}_0+4\pi^2\mathbf{n}^2/L^2)^{-2}, \tag{11}$$

where $\bar{r}_0=r_0+12u_0\langle\phi_0^2\rangle_0$, and now $\sum'$ means summation over all integers n_j except $n_1=\cdots=n_d=0$. The main difference can be absorbed in the shifted variable $\tilde{r}_0^0=\hat{r}_0+\tilde{d}\pi^2/L^2$ by our rewriting

$$S_{\mathrm{Dbc}}(\hat{r}_0,L)=S_{\mathrm{pbc}}(\tilde{r}_0^0,L)+L^{4-d}g(\tilde{r}_0^0L^2), \tag{12}$$

where $g(t)$ is a smooth function with finite limits $g(0)=-0.0084$ for $d=4$ and $g(\infty)=0$. We decompose S_{pbc} as previously,[9,10]

$$S_{\mathrm{pbc}}(\tilde{r}_0^0,L)=\int_q(\tilde{r}_0^0+q^2)^{-2}+G_{\mathrm{pbc}}(\tilde{r}_0^0L^2). \tag{13}$$

In $d=4-\epsilon$ the bulk integral yields[7] $A_d[\epsilon^{-1}-\frac{1}{2}+\frac{1}{2}\ln\tilde{r}_0^0+O(\epsilon)]$ with the crucial difference that $\ln\tilde{r}_0^0$ has replaced $\ln r_0$. This demonstrates that the shifted variable $r_0+\tilde{d}\pi^2/L^2$ discussed recently[11] should be maintained (and modified by $r_0\to\hat{r}_0$) *beyond mean-field theory.* We anticipate that higher loops yield powers of $\ln\tilde{r}_0^0$. These results suggest the introduction of a shifted renormalized temperature variable $\tilde{r}=Z_r^{-1}\times(r_0-r_{0c})$ with the usual bulk Z_r and $r_{oc}(u_0,L)=-\tilde{d}\pi^2/L^2+O(u_0)$. We choose to determine the $O(u_0)$ term by requiring that the total coefficient $\hat{\chi}_0(r_0,L)^{-1}$ of the $\phi_{\mathbf{1}}^2$ term of $H_1(\phi_1)+\Gamma(\phi_{\mathbf{1}}^2)$ vanishes at $r_0=r_{0c}$. This implies up to $O(u_0)$ (and for general n)

$$r_{0c}(u_0,L)=-\tilde{d}\pi^2L^{-2}-\tfrac{1}{3}(n+2)L^{-d}\times\mathrm{Tr}(\partial\ln A/\partial\phi_{\mathbf{1}}^2)+O(u_0^2), \tag{14}$$

where the matrix A is given by Eq. (7) and the derivative is taken at $\phi_{\mathbf{1}}^2=0$ and $r_0=r_{0c}$. It is our conviction that an L-dependent shift of r_0 can be incorporated in a fully renormalized theory. So far we have checked the consistency of Eq. (14) within an explicit calculation of the specific heat for Dbc up to one-loop order. By contrast, there exists no need for a shift of r_0 in case of pbc, at least up to two-loop order, within a dimensionally regularized theory.[12]

Equation (14) corresponds to a shifted reference temperature,

$$T_c(L)=T_c(\infty)\{1+[r_{0c}(u_0,L)-r_{0c}(u_0,\infty)]\xi_0^2\}, \tag{15}$$

with ξ_0 being the bulk-correlation-length amplitude (equal to 1.43 Å for ^{4}He). Note that $\hat{\chi}_0$ is not the true physical susceptibility. Therefore, $T_c(L)$ constitutes an intrinsic semimacroscopic quantity which differs fundamentally from the macroscopic "pseudocritical" temperatures (e.g., the position of the maximum of a thermodynamic quantity) defined previously.[1,2] In particular our $T_c(L)$ does not scale with the bulk correlation length. The shift $T_c(\infty)-T_c(L)$ can be regarded as a smooth correction to scaling which for $L\to\infty$ vanishes more rapidly than $L^{-1/\nu}$. (This correction is distinctly different from the usual Wegner corrections to scaling.) A fully quantitative calculation of r_{0c} itself requires a description that includes the cutoff. Nevertheless, dimensional regularization can be used in determining the shift $r_{0c}(u_0,L)-r_{0c}(u_0,\infty)$.

Application of the renormalization group leads to finite-size scaling functions $F(\tilde{t}L^{1/\nu})$ that depend on the L-dependent "scaling field"[13] $\tilde{t}=[T-T_c(L)]/T_c(\infty)$ rather than on $t=[T-T_c(\infty)]/T_c(\infty)$. This implies that $T_m(L)$ should satisfy Eq. (3) rather than Eq. (2).

In order to test our theory we have performed a one-loop calculation of the specific heat C_ϕ. The explicit (rather lengthy) expressions will be given elsewhere. In the application of these results we have employed an equivalent representation of the specific heat[14] $C=\chi_m+\gamma_0^2\chi_m^2C_\phi$ which after multiplicative renormalization is determined by the known effective renormalized couplings $\gamma(l)$ and $u(l)$.[7] Here an appropriate determination of the flow parameter $l(\tilde{t},\xi_0L^{-1})$ has to be made. As a consequence of having introduced $\tilde{r}$ and from the integration of the renormalization-group equation,[7] the asymptotic ($L^{-1}\to0,\tilde{t}\to0$) scaling relation

$$l(\tilde{t},\xi_0/L)=(\xi_0/L)f(L/\xi_0\tilde{t}^{-\nu}) \tag{16}$$

follows, where ν is the bulk exponent. With the overall amplitude of C identified from bulk data[8] we arrive at a quantitative description of the specific heat of confined ^{4}He along the λ line without further adjustments. For simplicity we have modeled the pore geometry (of diameter L) by a cube with Dbc in $\tilde{d}=2$ directions and pbc in $d-2$ directions.

For comparison we have also calculated C in the case of pbc ($\tilde{d}=0$, denoted by C_{pbc}). In Fig. 1 our results are compared with the data[3] of ^{4}He in the region $T \gtrsim T_m$ for the example $L=1000$ Å. The improvement of C_{Dbc} (solid lines) compared to C_{pbc} (dashed lines) is striking. In contrast to C_{pbc}, C_{Dbc} approaches the bulk (dot-dashed) curve *from below*—in agreement with the experiment. The main part of the large reduction of the maximum of C_{Dbc} can be traced to the enhancement factor $(\frac{3}{2})^{\tilde{d}}$ in $\tilde{u}_0$ of Eq. (5). Another conspicuous difference manifests itself in the (reduced) rounding temperature[1,2] $t^* = [T^*(L) - T_\lambda]/T_\lambda$. If one defines t^* to be the temperature where the deviation from the bulk curve is, say, 1%, then our t^*_{Dbc} is 2 orders of magnitude larger than T^*_{pbc}, i.e., $\xi(t^*_{\mathrm{Dbc}}) \ll L$. Again this is in agreement with the experimental data [Fig. 1(b)]. We consider the gradual (algebraic rather than exponential) approach to the bulk curve as the reason for the previous difficulty[3] in determining the rounding exponent θ. We interpret this as a surface effect induced by the Dbc. Note that these aspects of our theory are insensitive to the appropriate determination of $T_c(L)$. For $L=300$, 800, and 2000 Å we have found similar agreement between our theory (with Dbc) and experiment.[3] Further tests of our theory could be provided by specific-heat measurements at higher pressures.

We may now return to Eqs. (2) and (3) by using theoretical values for both T_c and T_m. Then it is a direct consequence of Eq. (16) that Eq. (3) contains the bulk $\nu=0.67$. In order to compare the L dependence of our T_m with experiment we have plotted $T_\lambda - T_m(L)$ double logarithmically versus L according to Eq. (2). The slope in the range 300 Å $\le L \le$ 2000 Å yields $\nu=0.60$, in good agreement with the apparent exponent $\nu=0.583 \pm 0.046$ of the data.[3] This resolves an apparent failure of scaling theory[1] that has been considered as a particularly disquieting problem in the theory of finite-size effects.[2]

The theoretical absolute values of $T_\lambda - T_m$ and of the height of the specific-heat maxima are somewhat smaller than the experimental values. Two reasons are as follows: First, the convergence of our perturbation expansion deteriorates near T_m and breaks down below T_m [since there the codiagonal elements of A change from $O(u_0^{1/2})$ to ~ 1]; second, we have not yet included the correct geometry of the cylindrical pores ($L_z \gg L \equiv L_x = L_y$). The breakdown well below T_λ was expected because higher modes become increasingly important. This does not touch on the reliability of our results for $T \gtrsim T_m$ where the sinusoidal (lowest mode) order-parameter profile is an appropriate approximation.

In conclusion, our findings indicate that the existing

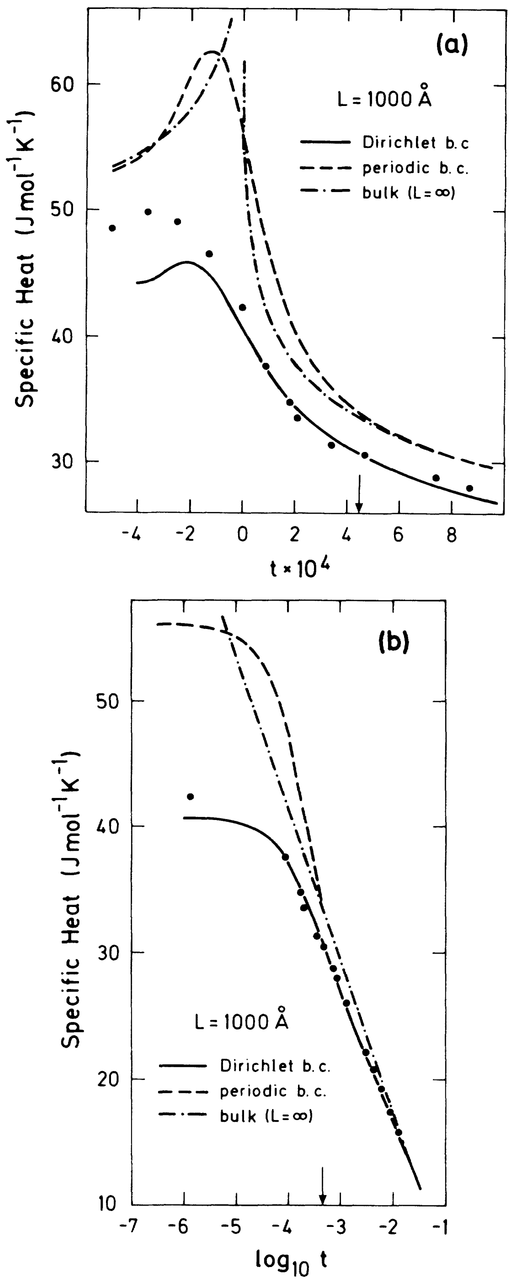

FIG. 1. (a),(b) Theoretical specific heat of confined ^{4}He (system size $L=1000$ Å) vs $t=(T-T_\lambda)/T_\lambda$ and $\log_{10} t$ for Dirichlet boundary conditions (solid lines) and for periodic boundary conditions (dashed lines). Data (dots) from Ref. 3; dot-dashed lines (bulk specific heat) from Ref. 8. The arrows indicate the reduced rounding temperature t^*_{pbc}.

data on the specific heat in confined ^{4}He can be reconciled with the theory in a natural way provided that the effect of realistic boundary conditions is taken into account. At the present level of accuracy our results support the assumption of $\psi=0$ near the walls (but certainly do not exclude a small finite value $|\psi| \ll |\psi|_{\mathrm{bulk}}$ of the coarse-grained order parameter and the possible relevance of a surface enhancement term to be studied in a more refined theory). Our present calculation does not yet explain the detailed L dependence of the height of the specific-heat maximum.[5] This may be due to the multimode problem[11] that one encounters in the crossover to the bulk behavior below T_λ.

An extension of the present theory to the superfluid density ρ_s would be of considerable interest. More precise measurements of ρ_s would also be highly desirable.

Finally we propose to apply our theory to the case $n=1$ in order to reanalyze numerical results for the Ising model with free edges[15] where deviations from the finite-size scaling prediction have also been seen. We suggest that these deviations are in part due to effects similar to those identified in the present paper. It remains to be seen to what extent the Dbc of the coarse-grained continuum model, Eq. (1), can be simulated by lattice models with free boundary conditions.

We would like to thank F. M. Gasparini for providing us with the data of Ref. 3 in numerical form.

[1]M. E. Fisher, in *Critical Phenomena,* International School of Physics "Enrico Fermi," Course 51, edited by M. S. Green (Academic, New York, 1971).

[2]For reviews see M. N. Barber, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983), Vol. VIII; K. Binder, Ferroelectrics **73**, 43 (1987).

[3]T. P. Chen and F. M. Gasparini, Phys. Rev. Lett. **40**, 331 (1978).

[4]F. M. Gasparini, G. Agnolet, and J. D. Reppy, Phys. Rev. B **29**, 138 (1984).

[5]F. M. Gasparini, T. P. Chen, and B. Bhattacharyya, Phys. Rev. B **23**, 5797 (1981).

[6]F. M. Gasparini and S. Mhlanga, Phys. Rev. B **33**, 5066 (1986).

[7]V. Dohm, Phys. Rev. Lett. **53**, 1379 (1984), and Z. Phys. B **60**, 61 (1985); R. Schloms and V. Dohm, Europhys. Lett. **3**, 413 (1987).

[8]G. Ahlers, Phys. Rev. A **3**, 696 (1971).

[9]E. Brézin and J. Zinn-Justin, Nucl. Phys. **B257 [FS14]**, 867 (1985).

[10]J. Rudnick, H. Guo, and D. Jasnow, J. Stat. Phys. **41**, 353 (1985).

[11]J. Rudnick, G. Gaspari, and V. Privman, Phys. Rev. B **32**, 7594 (1985).

[12]We have found that the "L-dependent mass shift" of $O(u^2)$ introduced by H. Guo and D. Jasnow, Phys. Rev. B **35**, 1846 (1987), is due to a computational error in their work. We thank D. Jasnow for confirming agreement with our calculation.

[13]The general possibility of smoothly L-dependent scaling fields was mentioned briefly by V. Privman and M. E. Fisher, J. Phys. A **16**, L295 (1983), but no specification was given under which conditions this possibility might arise.

[14]Strictly speaking our theoretical C should be interpreted as the specific heat at given chemical potential and given volume.

[15]T. W. Capehart and M. E. Fisher, Phys. Rev. B **13**, 5021 (1976); D. P. Landau, Phys. Rev. B **14**, 255 (1976).