Vortex-Loop Phase Transitions in Liquid Helium, Cosmic Strings, and High-T_c Superconductors

Gary A. Williams
Department of Physics and Astronomy, University of California, Los Angeles, California 90095
(Received 24 July 1998)

The distribution of thermally excited vortex loops near a superfluid phase transition is calculated from a renormalized theory. The number density of loops with a given perimeter is found to change from an exponential decay with increasing perimeter to an algebraic decay as T_c is approached, in agreement with recent simulations of both cosmic strings and high-T_c superconductors. Predictions of the value of the exponent of the algebraic decay at T_c and of the critical behavior in the vortex density are confirmed by the simulations, giving strong support to the vortex-folding model proposed by Shenoy. [S0031-9007(99)08401-X]

PACS numbers: 64.60.Cn, 11.27.+d, 67.40.Vs, 74.20.–z

The role of thermally excited vortex loops in three-dimensional phase transitions, where a U(1) symmetry is broken, has recently become a prime topic in cosmology [1,2] and high-T_c superconductivity [3–5]. These transitions are in the same universality class as the superfluid λ transition in ^{4}He. In the helium case our original renormalization theory based on vortex loops [6,7] has been extended to calculations of the specific heat [8] and to the dynamics of the transition [9]. In this theory the Landau-Ginzburg-Wilson Hamiltonian is rewritten to cast it in terms of its elementary excitations, spin waves and vortex loops, providing an alternative method for carrying out the renormalization process, compared to the more traditional perturbation theories which expand the Hamiltonian expressed in terms of the order parameter.

Here we further employ the loop theory to gain insight into recent simulations of the high-T_c transition [4,5] and of cosmic-string phase transitions in the early universe [1,2]. The probability of occurrence of a vortex loop with perimeter P is calculated and, in agreement with the simulations, we find a crossover from quasiexponential decay of the probability with the perimeter at low temperatures to purely algebraic decay precisely at T_c. This provides strong support for the phenomenological "Flory-scaling" treatment of the random-walking loops developed by Shenoy and co-workers [10].

In the vortex-loop theory the superfluid density ρ_s is reduced by thermally excited loops whose average diameter a increases as the temperature is increased, and the density is finally driven to zero at T_c by loops of infinite size [6]. Defining a dimensionless superfluid density by $K_r = \hbar^2 \rho_s a_0 / m^2 k_B T$, where m is the mass of the ^{4}He atom and a_0 is the smallest ring diameter, the equation for the renormalized density is given by [8]

$$\frac{1}{K_r} = \frac{1}{K_0} + A_0 \int_{a_0}^{a} \left(\frac{a}{a_0}\right)^6 \exp\left(-\frac{U(a)}{k_B T}\right) \frac{da}{a_0}. \quad (1)$$

Here $A_0 = 4\pi^3/3$, K_0 is the "bare" superfluid density resulting from the spin waves (and is the initial value of K_r), and $U(a)$ is the renormalized energy of a ring, given by

$$U(a)/k_B T = \pi^2 \int_{a_0}^{a} K_r \left[\ln\left(\frac{a}{a_c}\right) + 1\right] \frac{da}{a_0} + \pi^2 K_0 C, \quad (2)$$

where C is a nonuniversal constant characterizing the core energy. For helium C and a_0 are determined from two experimental inputs, $T_c = 2.172$ K and the amplitude of the superfluid density [8], yielding $C = 1.03$ and $a_0 = 2.5$ Å. The effective core size a_c in Eq. (2) was suggested by Shenoy and co-workers [7,10] to be a result of the random walk of the loop giving rise to radial fluctuations of order a_c about the average diameter. This folding of the loop occurs because antiparallel vortex segments lower the energy. A simple polymer-type calculation [10] using energy-entropy arguments yields $a_c/a = (K_r a/a_0)^\theta$, where $\theta = d/(d+2) = 0.6$ in $d = 3$ dimensions has the same form as the well-known Flory exponent of the self-avoiding walk.

Equations (1) and (2) then constitute a coupled set of integral equations for the renormalized superfluid density, and can be solved recursively starting from the bare scale a_0 and iterating to distances greater than the correlation length $\xi = a_0/K_r$. In practice these are converted to a set of coupled differential equations similar to the Kosterlitz recursion relations [11] for the two-dimensional case, and are solved using a Runge-Kutta technique [9]. As T is increased (K_0 decreased) the solution for ρ_s falls to zero as $(T_c - T)^\nu$, with $\nu = 0.6717$ for $\theta = 0.6$. This can be better matched to the most precise experimental value [12] $\nu = 0.6705$ by adjusting to $\theta = 0.594$, which is reasonable since it is known that the Flory-type arguments are not exact in three dimensions [13].

The arguments of Ref. [10] also yield a result for the average perimeter of a loop of diameter a,

$$\frac{P}{a_0} = B\left(\frac{a}{a_0}\right)^{1/\delta}, \quad (3)$$

where B is a constant and the exponent $\delta = 2/(d+2) = 0.4$. This form for the perimeter was at least partially verified in the computer simulations of Ref. [10], and in the XY model simulations of Epiney [14]. For P/a_0 greater than about 20 the Epiney data for the average loop size versus average perimeter can be fit by Eq. (3) with $B = 1.8$, although the resolution is poor because of scatter in the data resulting from the relatively small lattice (16^3) that was simulated.

The distribution of the density of loops with a given perimeter P can be obtained from the theory outlined above, which is of interest because these distributions have now been measured in the cosmic string [2] and high-T_c [4,5] simulations. The probability per unit volume for finding a loop of mean diameter between a and $a + da$ is

$$\frac{\pi}{2a_0^3}\left(\frac{a}{a_0}\right)^2 \exp\left(-\frac{U(a)}{k_BT}\right)\frac{da}{a_0}\,. \tag{4}$$

Equating this to the probability $D(P)dP/a_0$ of finding the corresponding loop of perimeter between P and $P + dP$ gives the probability distribution

$$D(P) = \frac{\pi}{2a_0^3}\,\frac{\delta}{B}\left(\frac{a}{a_0}\right)^{(3\delta-1)/\delta} \exp\left(-\frac{U(a)}{k_BT}\right). \tag{5}$$

For temperatures well below T_c, $U(a) \sim a\ln a$, and hence $D(P)$ decreases exponentially with P^δ. Near T_c, however, the behavior is quite different. By differentiating Eq. (1) with respect to a and substituting for the exponential term in Eq. (5) we get

$$D(P) = \frac{\pi}{2a_0^3}\,\frac{\delta}{B}\left(\frac{a}{a_0}\right)^{-(3\delta+1)/\delta}\left(\frac{\partial(1/K_r)}{\partial a}\right). \tag{6}$$

Precisely at T_c, K_r from Eq. (1) satisfies the condition $K_r a/a_0 = D_0 = 0.39$, at least for values of a greater than about $5a_0$, and where D_0 is a universal constant [8,15]. This condition is the three-dimensional equivalent of the univeral "jump" of the superfluid density in two dimensions [11]. Inserting this result into Eq. (6) and employing Eq. (3) yields the prediction that at T_c the loop distribution will cross over from exponential to algebraic decay with P,

$$D(P) = \frac{\pi\delta B^{3\delta}}{2a_0^3A_0D_0}\left(\frac{P}{a_0}\right)^{-\gamma}, \tag{7}$$

where the exponent $\gamma = 3\delta + 1$. For the "Flory" value $\delta = 0.4$ this would predict $\gamma = 2.2$. This form for $D(P)$ signals the onset of loops of infinite size, since they no longer have a vanishing probability. It should be noted that the algebraic decay is a consequence of the strong renormalization at T_c, where the screening of large loops by smaller ones causes the variation of $U(a)$ to change [9] from $\sim a\ln a$ to $\ln a$ at T_c, causing the change from Eq. (5) to Eq. (7).

The crossover from exponential to algebraic decay is a central feature observed in the recent cosmic-string [2] and high-T_c [4,5] simulations using lattices larger than 96^3, and was also seen with more limited resolution in the earlier XY model simulations of Epiney [14]. The results of Antunes and Bettencourt [2] yield $\gamma = 2.23 \pm 0.04$ at T_c, which from the analysis above gives $\delta = 0.41 \pm 0.01$, in very good agreement with Shenoy's Flory-scaling prediction. Fits to the high-T_c simulations of Nguyen and Sudbo [4] (in the zero-field, isotropic limit of their Villain model) give $\gamma = 2.4$ [16], leading to a higher value $\delta = 0.48$. However, the results of Ref. [2] show that γ increases rapidly above T_c to the value of 2.5 found by Vachaspati and Vilenkin [17], and hence an accurate determination requires bracketing temperatures very close to T_c. It is interesting that the result $\gamma = 3\delta + 1$ apparently remains valid even above T_c, since the Vachaspati-Vilenkin value of $\gamma = 2.5$ is based on the "Brownian" value $\delta = 0.5$.

The magnitude of the loop distribution $D(P)$ at T_c as calculated from either Eq. (5) or (7) appears to be about a factor of 3 smaller than that found in the simulations. Comparing the continuum calculation to the lattice results is made difficult by uncertainties in matching at the scale of the lattice spacing a_l; in computing the magnitude of Eq. (7) for the comparison, the geometric value $a_0 = \sqrt{2}\,a_l$ was employed, but it is not entirely clear that this is the correct choice.

The total length per unit volume ρ_v of the vortex loops can be found by multiplying $D(P)$ by P and integrating. At T_c this can be found explicitly using Eq. (7),

$$\rho_v(T_c) = \frac{\pi\delta B}{2a_0^2A_0D_0(3\delta - 1)}\,. \tag{8}$$

The quantity $\rho_v(T_c)a_l^2$ was postulated in Ref. [1] to be universal, with a value of 0.6 in lattice units (0.2 per placquette, with three placquettes per unit volume). This means that the coefficient B in Eq. (8) characterizing the relationship between the perimeter and the average loop diameter must be universal, since all of the other parameters are. As with $D(P)$ above, the magnitude of Eq. (8) must be multiplied by a factor of about 3 to match with the lattice results. For liquid helium, the vortex density [18] at T_c is then about $1/a_0^2 \sim 1 \times 10^{15}$ cm^2, which is many orders of magnitude higher than previous estimates [19] which did not use a renormalized theory.

A further prediction of the loop theory is the existence of critical behavior in the vortex density at T_c [18], which has now been seen in the cosmic-string simulations [1]. This is shown in Fig. 1, which plots the normalized density versus T_c/T, calculated by integrating Eq. (5) very near the transition. The behavior above T_c (dashed lines) is only conjectured, as the theory is not valid there. To suppress the exponential variation arising from thermal excitation of the smallest loops, the core energy constant was taken to be the relatively large value $C = 4/3$, corresponding to the Villain model. The density just below T_c is found to decrease from its value at T_c as $-(T_c - T)^\delta$. This exponent was not measured in the cosmic-string simulations, probably because of the relatively low core

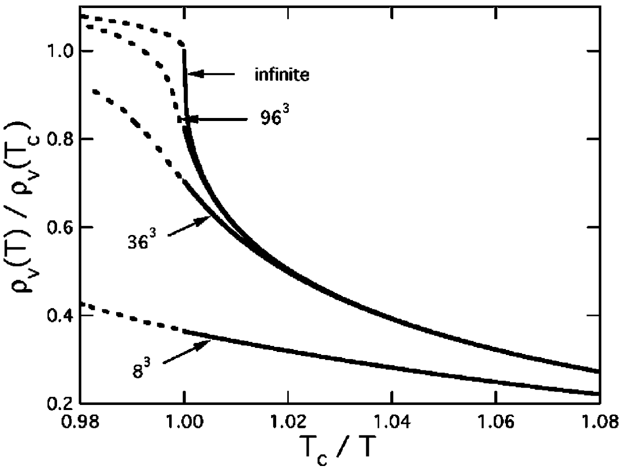

FIG. 1. Normalized vortex density as a function of T_c/T, for several different lattice sizes.

energy in that model, which would make it difficult to separate the algebraic behavior from the exponential. However, the exponent of the density in the region just above T_c was measured in Ref. [1] to be 0.39 ± 0.01, which is quite consistent with the value of $\delta = 0.41$ determined above from the same type of simulation. It is well known from scaling and renormalization-group studies that many critical exponents are identical above and below the transition, and it is likely that this exponent constitutes a further measurement of δ. Since δ is less than 1, T_c marks an inflection point in the density, where the curvature changes sign.

Also shown in Fig. 1 is the effect of a finite-size lattice on the density near T_c. For this the recursion relations are stopped at a finite scale that is a fraction $\beta = 0.75$ smaller than the lattice size, where β was found in Ref. [8] by comparing it to the helium simulations of Ref. [15]. The effect of finite size is to smear out the critical behavior, and this explains why it was not apparent in the early simulations [20], which only used a maximum 10^3 lattice size.

The coherence length in the loop theory can be identified with the diameter of the largest loop that is thermally excited [6]. Since this is divergent at T_c, in a system of finite (but macroscopic) size, the transition can be identified with the point where a loop just touches two opposing boundaries of the system. This is the percolation threshold for the establishment of the infinite vortex cluster, as first proposed by Onsager 50 years ago, and verified in simulations [21]. At higher temperature even larger loops can be excited; these can take the form of a single vortex line passing from one side of the system to the other, with the topological return path of the loop being around the outside of the system. These are known as "string" excitations in cosmology [1,2,17]. The leftover strings from the rapid cooling through the phase transitions in the early universe are thought to be the source of matter [19,22]. A laboratory example of this may be the observation of a few remnant vortex lines [23] in a finite-sized sample of liquid ^{4}He which has not been rotated or stirred, but simply cooled through the λ transition.

The key role of thermally excited vorticity in the present model of the phase transition allows a rather different viewpoint of the Kibble-Zurek mechanism [19,22] for defect formation in rapidly quenched transitions as discussed above. This is of interest because of the possibility of carrying out such experiments in liquid helium [19,22,24,25]. In this view, the vortices "created" in a quench of superfluid ^{4}He through T_c are simply a perturbation on the equilibrium vortex density. This perturbation is a consequence of the dynamics of large loops, which become slow in their response to external fields, and which are actually the source of the critical slowing down of the equilibrium transition [9]. In a rapid quench the large loops in the vicinity of T_c cannot keep up and fall out of equilibrium, forming an excess density that survives to lower temperatures, finally decaying to the equilibrium line density only after the quench is stopped. It may be possible to model this process analytically using the Fokker-Planck equation for the loop distribution function formulated in the dynamic theory of Ref. [9], with the temperature being a ramp function in time. It should be noted that the exponent δ from above plays an important role in the vortex dynamics, since the frictional drag force on a loop is proportional to its total perimeter. It was found in Ref. [9] that the dynamic exponent characterizing critical slowing down is given by $x = z\nu$, where $z = (1 - \delta)/\delta$. For the "Flory" value $\delta = 2/(d + 2)$ this gives the scaling result $z = d/2 = 3/2$; for $\delta = 0.41$ as found above, $z = 1.44$, a few percent smaller. The possibility of deviations from the scaling result has been suggested previously in perturbative dynamic theories [26].

Vortex creation has been observed in superfluid ^{3}He [25], where the quench is induced by absorbed neutrons depositing their energy in a small region of the liquid, which heats it above T_c, and which is then rapidly cooled back down by the surrounding cold liquid [25]. Although ^{3}He is a p-wave BCS superfluid, vortex loops will still be associated with the phase transition as above, but due to the Ginzburg criterion [27] they will only be appreciable in a very narrow temperature range near T_c, since the zero-temperature coherence length of ^{3}He is of order 500 Å, compared with $a_0 = 2.5$ Å in ^{4}He. The theory [25] of the quenched ^{3}He involves the exponents δ and γ at T_c; the use of the Brownian values [17] $\gamma = 2.5$ and $\delta = 0.5$ needs to be reexamined in light of the present results.

The vortex-loop model also allows insights into the high-T_c superconducting transition in zero field. If T_c is the point where the loops of infinite size act to bring all supercurrents to a halt, then it is *not* to be identified as the point where thermal deexcitation of Cooper pairs is complete. The continued existence of pairs above T_c has been suggested in experiments, commonly known as the pseudogap phenomenon [28]. The vortex loops constitute a concrete physical picture of the "phase fluctuations" postulated to give rise to this effect in Ref. [28]. The Cooper pairs above T_c will not be the same as those below, since they will no longer be part of a macroscopic BCS-type condensate, which is destroyed by the vortices. Presumably the pairs would be more localized excitations, on the scale of the 10–15 Å zero-temperature coherence length.

The vortices also offer a simple explanation [29] of the magnetic flux noise in YBCO samples that is observed to increase rapidly by many orders of magnitude over a temperature range of order 5 K near T_c [30]. When the loops being thermally excited terminate on the sample surface, they will induce dipolar current patterns on the surface, and this will generate magnetic flux that can be sensed by a detection loop above the surface. As T_c is approached from below both the number and size of the loops will increase, increasing the flux noise through the detector. This effect can also be observed in a low-T_c superconductor, since the same vortex-loop transition occurs also in that case, but with the considerable difference that the large zero-temperature coherence length (several thousand Å) causes the temperature range where the vortices are appreciable to be very much closer to T_c. The experiments [31] showed that indeed a very sharp flux-noise peak could be observed in a lead sample only within about 2 mK of T_c, and that this was only an upper limit to the width due to the resolution of the thermometry and the additional broadening that would be caused by a distribution of T_c's across the sample.

In summary, a vortex-loop theory is able to provide physical insight into recent models of cosmic strings and high-T_c superconductors. The theory relates the critical exponents measured in the simulations to the random-walk nature of the loops, and the good agreement between the predicted and measured exponents provides strong support for the Flory-scaling ansatz of Shenoy [7].

Useful correspondence with L. Bettencourt, J. Clarke, M. Hindmarsh, A. Sudbo, and G. Volovik is gratefully acknowledged. This work is supported by the U.S. National Science Foundation, Grants No. DMR 95-00653 and No. DMR 97-31523.

[1] N. Antunes, L. Bettencourt, and M. Hindmarsh, Phys. Rev. Lett. **80**, 908 (1998).
[2] N. Antunes and L. Bettencourt, Phys. Rev. Lett. **81**, 3083 (1998).
[3] S.R. Shenoy and B. Chattopadhyay, Phys. Rev. B **51**, 9129 (1995); D. Dominguez *et al.*, Phys. Rev. Lett. **75**, 717 (1995); M. Kiometzis, H. Kleinert, and A. Schakel, Phys. Rev. Lett. **73**, 1975 (1994); Z. Tesanovic, cond-mat/9801306.
[4] A. Nguyen and A. Sudbo, Phys. Rev. B **57**, 3123 (1998); **58**, 2802 (1998).
[5] S. Ryu and D. Stroud, Phys. Rev. B **57**, 14 476 (1998).
[6] G. A. Williams, Phys. Rev. Lett. **59**, 1926 (1987).
[7] S.R. Shenoy, Phys. Rev. B **40**, 5056 (1989).
[8] G. A. Williams, J. Low Temp. Phys. **101**, 421 (1995).
[9] G. A. Williams, Phys. Rev. Lett. **71**, 392 (1993); J. Low Temp. Phys. **93**, 1079 (1993).
[10] B. Chattopadhyay, M. Mahato, and S.R. Shenoy, Phys. Rev. B **47**, 15 159 (1993).
[11] D. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. **39**, 1201 (1977).
[12] L. Goldner and G. Ahlers, Phys. Rev. B **45**, 13 129 (1992).
[13] N. Madras and A. Sokal, J. Stat. Phys. **50**, 109 (1988).
[14] J. Epiney, Diploma thesis, ETH Zurich, 1990 (unpublished).
[15] The quantity $D_0/\beta = 0.52$ is the universal number which should be compared with the value 0.49 found in the finite-size simulations of E. Pollack and K. Runge, Phys. Rev. B **46**, 3535 (1992).
[16] The authors of Ref. [4] originally claimed the value of the exponent to be 3, but they have now reported (private communication) that a value of 2.4 provides a better description of their data.
[17] T. Vachaspati and A. Vilenkin, Phys. Rev. D **30**, 2036 (1984).
[18] G. A. Williams, Z. Phys. B **98**, 341 (1995).
[19] A. Gill and T. Kibble, J. Phys. A **29**, 4289 (1996).
[20] G. Kohring, R. Shrock, and P. Wills, Phys. Rev. Lett. **57**, 1358 (1986).
[21] L. Onsager, Nuovo Cimento Suppl. **6**, 249 (1949); J. Akao, Phys. Rev. E **53**, 6048 (1996).
[22] W. Zurek, Phys. Rep. **276**, 177 (1996).
[23] D. Awaschalom and K. Schwarz, Phys. Rev. Lett. **52**, 49 (1984).
[24] M. Dodd *et al.*, Phys. Rev. Lett. **81**, 3703 (1998).
[25] G. Volovik, Czech. J. Phys. **46**, Suppl. S6, 3048 (1996); V. Ruutu *et al.*, Phys. Rev. Lett. **80**, 1465 (1998); C. Bäuerle *et al.*, Nature (London) **382**, 332 (1996).
[26] C. De Dominicus and L. Peliti, Phys. Rev. B **18**, 353 (1978).
[27] V. Ginzburg, Sov. Phys. Solid State **2**, 1824 (1960).
[28] V. Emery and S. Kivelson, Nature (London) **374**, 434 (1995).
[29] G. A. Williams, Physica (Amsterdam) **194B–196B**, 1415 (1994).
[30] M. Ferrari *et al.*, J. Low Temp. Phys. **94**, 15 (1994).
[31] J. Clarke (private communication).