EUROPHYSICS LETTERS 1 June 2002

Europhys. Lett., **58** (5), pp. 705–711 (2002)

Critical exponent η_ϕ of the lattice London superconductor and vortex loops in the 3D XY model

P. Olsson

Department of Theoretical Physics, Umeå University - 901 87 Umeå, Sweden

(received 1 February 2002; accepted 5 March 2002)

PACS. 64.60.Cn – Order-disorder transformations; statistical mechanics of model systems.
PACS. 74.40.+k – Fluctuations (noise, chaos, nonequilibrium superconductivity, localization, etc.).
PACS. 64.60.Fr – Equilibrium properties near critical points, critical exponents.

Abstract. – The anomalous dimension of the lattice London superconductor is determined from finite-size scaling of the susceptibility to be $\eta_\phi = -0.79(1)$. It is furthermore found that the vanishing of the vortex loop line tension in the 3D XY model, which should be related to that exponent, agrees reasonable well with this value of η_ϕ. Deviations from this behavior are however also identified and it is suggested that they are an effect of the vortex loop intersections and therefore will vanish only in the limit of low vortex density.

The properties of the Meissner transition is a classical problem in statistical physics. Whereas this transition was originally believed to always be of first order, the work by Dasgupta and Halperin [1] gave strong arguments that the transition should instead be continuous. The argument is based on a duality transformation of the lattice London superconductor (LLS) and suggests that the transition should be 3D XY-like, but with the temperature scale inverted. A direct consequence of this relation is the expectation that the correlation length exponent ν should be the same in the superconductor as in the 3D XY (planar rotor) model. However, with fluctuations in both the phase angle and the gauge field, it becomes possible to define two characteristic lengths, and the behavior of the magnetic screening length λ has recently been a subject of some controversy [2, 3]. The current evidence [4, 5] points to a scenario where both characteristic lengths diverge with the same exponent. This is related to the presence of an anomalous dimension $\eta_A = 1$ for the gauge fluctuations [3].

What is needed beside ν and η_A for the characterization of the universality class of the transition is a knowledge of the anomalous dimension η_ϕ associated with the phase correlations. This quantity was determined to be $\eta_\phi = -0.20$ from a renormalization group calculation to one loop order [3]. Determinations from simulations have so far only been indirect through the properties of vortex loops in the 3D XY model [5–7]. The main motivation for these analyses was the possible connection between the sign of η_ϕ and the existence of a vortex loop blowout transition in high-T_c superconductors in applied magnetic fields [6, 8].

In this letter we report on a direct determination of the anomalous dimension η_ϕ from Monte Carlo (MC) simulations of the LLS that gives a surprisingly large negative value,

$\eta_\phi = -0.79 \pm 0.01$. We also consider in detail the approach to determine this exponent from the properties of the vortex loops in the 3D XY model. The conclusion from that study is that there is a reasonable agreement with the expected behavior, but also some deviations close to criticality. It is argued that these deviations are due to vortex loop intersections and therefore will vanish only in the limit of low vortex density.

The Hamiltonian of the LLS [1,4] is

$$H = \sum_{i\mu} \left\{ U(\theta_{i+\hat{\mu}} - \theta_i - A_{i\mu}) + \frac{1}{2} J \lambda_0^2 [\boldsymbol{D} \times \boldsymbol{A}]_{i\mu}^2 \right\}, \tag{1}$$

where θ_i is the phase of the superconducting wave function on site i and $A_{i\mu}$ is the vector potential on the link starting at site i and pointing along $\hat{\mu}$. The sum is over all bonds of a 3D simple cubic lattice of unit grid spacing and $\mu = x, y, z$. In the first term, the kinetic energy of flowing supercurrents, $U(\varphi)$ is the Villain function [9]

$$e^{-U(\varphi)/T} = \sum_{p=-\infty}^{\infty} e^{-J(\varphi - 2\pi p)^2/(2T)}. \tag{2}$$

In the second term, the magnetic-field energy, λ_0 is the bare magnetic penetration length and $\boldsymbol{D} \times \boldsymbol{A}$ is the discrete circulation of the vector potential.

In our simulations we chose $\lambda_0 = 0.3$ to be able to compare with ref. [4] and fix the gauge through $\boldsymbol{D} \cdot \boldsymbol{A} = 0$ to facilitate a simple determination of the spin correlations. The spin correlations defined here in the Landau gauge are identical to gauge-invariant correlations which display long-range order below the transition [10]. To fulfill this constraint we update the $A_{i\mu}$ by simultaneously adding δA to four $A_{i\mu}$ around an elementary plaquette, a procedure which was also used in ref. [7]. We perform our MC simulations with the standard Metropolis algorithm, first sweeping sequentially through the phase angles θ_i and then sweeping three times with attempts to change the circulation of $\boldsymbol{A}$ in the three different directions. The length of the runs close to T_c were at least 10^7 sweeps through the lattice, but often much longer. The measured quantities discussed here are the second and fourth moment of the magnetization,

$$m^p = \left| \frac{1}{L^3} \sum_i e^{i\theta_i} \right|^p,$$

which are used to obtain the dimensionless fraction

$$Q = \frac{\langle m^2 \rangle^2}{\langle m^4 \rangle}, \tag{3}$$

similar to Binder's cumulant, which is used to determine T_c. The susceptibility at the transition is obtained from the standard relation $\chi = L^3 \langle m^2 \rangle$.

The critical temperature for the LLS with the same parameter, $\lambda_0 = 0.3$, has already been determined with high precision [4]. Our present analysis of Q, therefore, mainly serves to confirm that the critical properties may be correctly determined from our simulations with $\boldsymbol{D} \cdot \boldsymbol{A} = 0$. Figure 1(a) shows Q *vs.* temperature for system sizes $L = 8$, 12, 16, and 24. We find that the curves for $L > 8$ cross at $T \approx 0.80$. The $L = 8$ data does however not cross the other curves at the same temperature, a typical sign of corrections to scaling. This data is therefore not included in the scaling collapse. To get a more precise determination of T_c we use all our data for $12 \leq L \leq 32$ in a narrow range around T_c, $|tL^{1/\nu}| < 1.1$, and assume the scaling form $Q(t, L) = f_Q(tL^{1/\nu})$, where $t = T/T_\mathrm{c} - 1$, and $f_Q(x)$ is a scaling function.

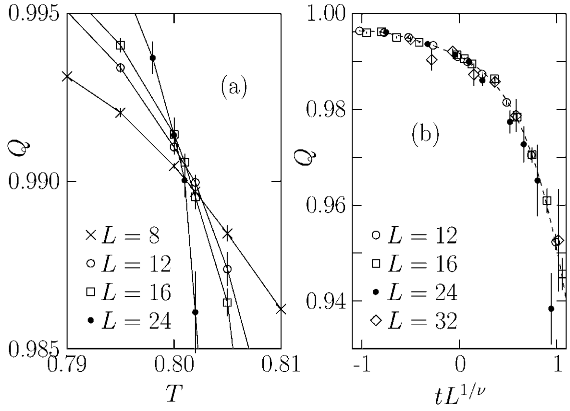

Fig. 1 – Determination of T_c from the crossing of Q given by eq. (3). Panel (a) shows data for $L = 8$ through 24; the $L = 8$ data lies below the crossing point. Panel (b) shows the scaling collapse for sizes $L = 12$ through 32.

We fix $\nu = 0.672$ [11] and let $f_Q(x)$ be a fifth-order polynomial in x. The data collapse nicely, fig. 1(b), and we find $T_c = 0.800 \pm 0.001$ in good agreement with $T_c = 0.8000 \pm 0.0002$ from ref. [4]. Repeating the analysis with ν as a free parameter we obtain $\nu = 0.70 \pm 0.04$, $T_c = 0.800 \pm 0.001$.

To determine the anomalous dimension η_ϕ we make use of the standard finite-size scaling relation $\chi(T_c, L) \sim L^{2-\eta_\phi}$. The susceptibility at $T_c = 0.8$ is shown in fig. 2(a). The points do indeed to an excellent approximation fall on a straight line and using data for $L \geq 12$ we obtain $\eta_\phi = -0.79 \pm 0.01$. Figure 2(b) shows a determination of the exponent β from the temperature dependence of $\langle m^2 \rangle$. This data is for temperatures at which we expect the finite-size effects to be negligible. The result is $\beta = 0.069 \pm 0.003$ in good agreement with what we expect from η_ϕ: $\beta = \frac{1}{2}\nu(d - 2 + \eta_\phi) = 0.070 \pm 0.003$.

We now turn to the alternative and indirect approach to determine η_ϕ through the behavior of the dual model which is the ordinary 3D XY model [1]. The idea [6] is that the vanishing

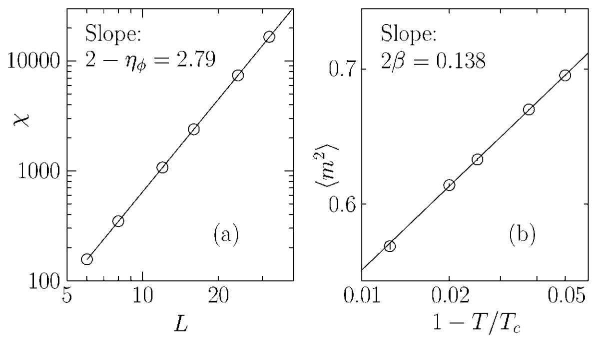

Fig. 2 – Panel (a) shows a finite-size scaling of the susceptibility at $T_c = 0.8$. The data fits nicely to a line with slope $2 - \eta_\phi = 2.79$. Panel (b) shows the determination of the exponent β from the T-dependence of $\langle m^2 \rangle$ for $L = 64$.

of the line tension of the vortex loops (see below) as $T \to T_c^-$ is governed by γ_ϕ,

$$\epsilon \sim (1 - T/T_c)^{\gamma_\phi}, \tag{4}$$

which is related to η_ϕ through the Fisher scaling relation $\gamma_\phi = \nu(2 - \eta_\phi)$. The basis for eq. (4) is the connection between the field theory that corresponds to the LLS and a gas of interacting loops [6,12,13]. Whereas this less direct determination of η_ϕ of course is more prone to errors, it is interesting to examine if the same value of η_ϕ can be obtained in that way. We will in the following examine the vanishing of ϵ for two different cases and also comment on the analysis in ref. [6] that gave $\eta_\phi \approx -0.18$.

The standard way to locate vortices in a XY model is from the angular difference $\varphi_{ij} = \theta_i - \theta_j$ between nearest neighbors, with $|\varphi_{ij}| < \pi$. For each plaquette the vorticity is then obtained from

$$n = \frac{1}{2\pi}(\varphi_{12} + \varphi_{23} + \varphi_{34} + \varphi_{41}). \tag{5}$$

Since the Villain interaction, eq. (2), essentially is a harmonic interaction where vortices are included through the integers p_{ij}, vorticity may also be defined through these integers as $n = p_{12} + p_{23} + p_{34} + p_{41}$. The p_{ij} need, however, not be included in the simulations. For each link we instead first calculate $\varphi_{ij}^0 = \theta_i - \theta_j$ and then probabilistically set the angular difference to $\varphi_{ij} = \varphi_{ij}^0 - 2\pi p_{ij}$, where p_{ij} is an integer chosen with the relative weight $e^{-J(\varphi_{ij}^0 - 2\pi p_{ij})^2/(2T)}$. The vorticity is then calculated from eq. (5). These vortices are exactly identical to the vortex lines in the dual vortex line model. The density of these dual vortices (DV) turns out to always be higher than the density of standard vortices (SV).

The simulations of the 3D XY model were performed with the Wolff cluster update method and Villain interaction (*i.e.*, eq. (1) neglecting the $A_{i\mu}$) on a cubic lattice with $L = 128$. The average for each data point is based on typically 10^5 measurements. The simulations were performed with both SV and DV discussed above. The tracing-out of vortex loops was done by always choosing the path randomly when two (or more) vortex loops meet at an elementary cube.

After identifying the vortex loops we measure the perimeter p of each such loop. The distribution $D(p)$ is then calculated from these values.

The line tension ϵ is obtained by fitting [6]

$$D(p) \propto p^{-\alpha} \exp[-\epsilon p/T], \tag{6}$$

with α, ϵ and a prefactor as free parameters. To get good-quality fits we only used data for large perimeters, $p > 0.8T/\epsilon$. Figure 3 shows the line tension ϵ determined with both SV and DV. Note that we are here examining a very narrow temperature region to be able to probe the behavior in the critical region; most data points are within a few percent below $T_c = 3.0024(1)$ [14]. With logarithmic scales on both axes the slope as $T \to T_c$ is expected to give the exponent γ_ϕ. To facilitate a comparison with the above-obtained $\eta_\phi = -0.79$ we draw two solid lines in fig. 3(a) that correspond to $\gamma_\phi = \nu(2 - \eta_\phi) = 1.87$. As seen in the figure, the data points are in reasonable agreement with this prediction. The indirect method based on the distribution of vortex loop diameters is thus found to give results for η_ϕ which agree with what we found with the direct method.

A more detailed analysis, however, casts some doubts on this agreement. This is especially clear for the DV data, but a more detailed look at the SV data as in fig. 3(b) shows that the points start to bend down as T_c is approached. It would at first seem natural to ascribe this discrepancy to a finite-size effect as the size of the biggest loops starts to approach the size of

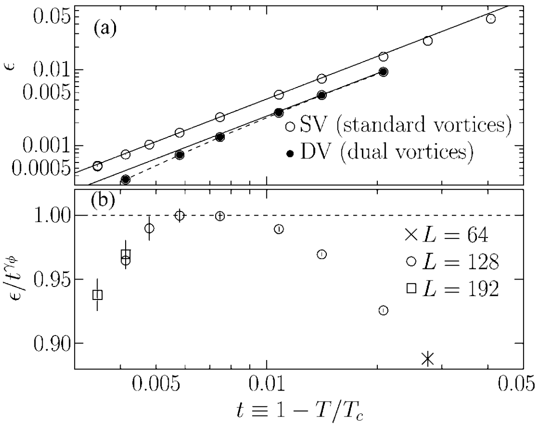

Fig. 3 – Panel (a) shows the line tension *vs.* reduced temperature from our analyses of the vortex loops. The agreement with the solid lines with slope $\gamma_\phi = 1.87$ appears to be rather good, but a closer look reveals significant deviations from this behavior. Panel (b) shows the deviation from the straight line in panel (a) for SV.

the system. This does, however, not turn out to be a tenable explanation: First, the results do not change markedly when increasing the system size; second, for the temperatures and lattice sizes in the figure there are no loops with the size approaching the system size, and finally, the effect of the finite size turns out to work in the opposite direction; it reduces the number of large loops and would thereby instead give too large a value for the line tension as $T \to T_c$.

We now suggest that the reason for this discrepancy is that things are messed up by the vortex loop intersections which are not accounted for in the theoretical considerations regarding vortex loops. One way to understand the effect of the intersections is through a Gedanken experiment:

1. Produce a set of vortex loops with the distribution $D_0(p) = \exp[\epsilon_0 p/T]$.
2. Throw them onto a lattice.
3. Apply the loop tracing algorithm.
4. Calculate a new $D(p)$ and determine ϵ from the decay of $D(p)$.

We will now argue that one would expect the obtained distribution to be different from the original one, $D(p) \neq D_0(p)$ and, more specifically, $\epsilon < \epsilon_0$. With a random tracing of vortex loops each intersection of two loops will, with 50% probability, make them merge to a single loop. The number of vortex loops will thus decrease and this implies that the average perimeter increases. With the assumption that the shape of the distribution remains the same this is only possible if the obtained line tension is smaller, $\epsilon < \epsilon_0$. This conclusion has been verified with simulations on a simplified version of the above Gedanken experiment. More details will be given elsewhere.

For each temperature we may assume that there is a bare distribution $D_0(p)$ characterized by $\epsilon_0(T)$ and that eq. (4) holds for $\epsilon_0(T)$. As discussed above, ϵ_0 is not directly accessible, but what we obtain after the random tracing is only $\epsilon < \epsilon_0$. This is a possible reason for the observed deviations from the expected behavior (solid lines) in fig. 3. Since the density

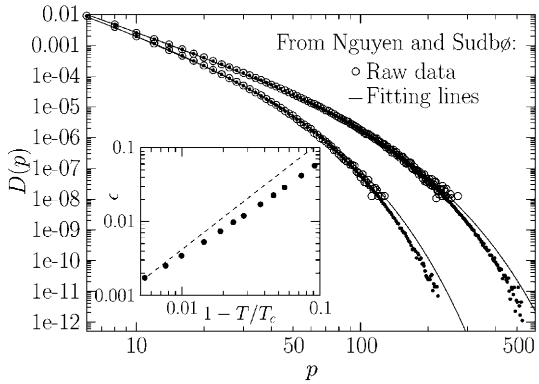

Fig. 4 – $D(p)$ for the 3D XY model with cosine interaction and splitting of self-intersecting loops. The fitting lines from [6] do not agree well with our more precise data (solid dots). The inset shows our values for ϵ; the slope is clearly different from $\gamma_\phi = 1.45$ (dashed line) obtained in ref. [6].

of intersections increases with increasing temperature, the drop of ϵ as T_c is approached is precisely what would be expected from this picture. The reason why the high-density data (DV) is far off, whereas the low-density data (SV) is fairly close to the expected behavior, is then the higher vortex density in the DV simulations. This, furthermore, suggests that the theoretically expected behavior of ϵ could at most be found in models with very low vortex density at criticality.

The determination of the line tension for vortex loops in a 3D XY model was first made in ref. [6]. Their simulations were with cosine spin interaction ($T_c \approx 2.2$) and a different method for tracing out the loops; self-intersecting vortex loops are always split into two. They found $\eta_\phi = -0.18 \pm 0.07$, in agreement with the analytically obtained $\eta_\phi \approx -0.2$ [3]. However, a comparison with our more precise MC data (now obtained with cosine interaction and splitting of intersecting loops) casts strong doubt on their analysis. Figure 4 shows our values for $D(p)$ (dots) together with both the data (open circles) and the fitting curves (solid lines) for $T = 2.0$ and 2.1 from ref. [6]. We first note that the two different sets of MC data agree well. From the large-p part of the data it is however clear that the fitting curves from ref. [6] do not agree with our data. The same discrepancy can actually also be seen for $T = 2.0$ in fig. 3 of ref. [6]. The inset in fig. 4 shows our values for ϵ obtained from a fit to eq. (6) only including data for $p > 1.2T/\epsilon$. The slope differs clearly from $\gamma_\phi = 1.45$ shown by the dashed line. We therefore conclude that the good agreement [6] with the analytically obtained $\eta_\phi \approx -0.2$ was only accidental. In our analysis the slope approaches $\gamma_\phi \approx 1.15$ as $T \to T_c$. If one instead uses the ordinary random loop tracing that allows for vortex loop intersections, the line tension is found to behave much the same as in fig. 3, with both a reasonable agreement with γ_ϕ as well as significant deviations close to criticality. This again shows the central role of the precise method for tracing out the loops and thereby the intersections for the vortex loop properties.

To conclude, our main result is a direct determination of the anomalous dimension in the LLS, giving $\eta_\phi = -0.79 \pm 0.01$. We have also attempted a determination of the same quantity from the vanishing of the line tension in the 3D XY model. We found a reasonable agreement when using random intersections but also concluded that this method cannot be used for precise determinations of the exponent. The reason is the presence of deviations close to T_c which we suggest to be due to the vortex loop intersections. This implies that the "correct" behavior as $T \to T_c$ can at most be expected in the limit of low vortex density.

* * *

The author thanks P. Minnhagen, A. Sudbø, A. Tanaka, S. Teitel and Z. Tešanović for valuable discussions. This work was supported by the Swedish Natural Science Research Council through Contract No. E 5106-1643/1999.

REFERENCES

[1] Dasgupta C. and Halperin B. I., *Phys. Rev. Lett.*, **47** (1981) 1556.
[2] Kiometzis M., Kleinert H. and Schakel A. M. J., *Phys. Rev. Lett.*, **73** (1994) 1975.
[3] Herbut I. F. and Tešanović Z., *Phys. Rev. Lett.*, **76** (1996) 4588.
[4] Olsson P. and Teitel S., *Phys. Rev. Lett.*, **80** (1998) 1964.
[5] Hove J. and Sudbø A., *Phys. Rev. Lett.*, **84** (2000) 3426.
[6] Nguyen A. K. and Sudbø A., *Phys. Rev. B*, **60** (1999) 15307.
[7] Hove J., Mo S. and Sudbø A., *Phys. Rev. Lett.*, **85** (2000) 2368.
[8] Tešanović Z., *Phys. Rev. B*, **59** (1999) 6449.
[9] Villain J., *J. Phys. (Paris)*, **36** (1975) 581.
[10] Kennedy T. and King C., *Phys. Rev. Lett.*, **55** (1985) 776.
[11] Hasenbusch M. and Török T., *J. Phys. A*, **32** (1999) 6361.
[12] Thomas P. R. and Stone M., *Nucl. Phys. B*, **144** (1978) 513.
[13] Kleinert H., *Gauge Fields in Condensed Matter*, Vol. **I** (World Scientific, Singapore) 1989, p. I.6.17.
[14] P. Olsson, unpublished.