

Monte Carlo calculation of the linear resistance of a three dimensional lattice Superconductor model in the London limit

Hans Weber¹ and Henrik Jeldtoft Jensen²

¹*Department of Physics, Luleå University of Technology, S-971 87 Luleå, Sweden*

²*Department of Mathematics, Imperial Collage, London SW7 2BZ, United Kingdom*

We have studied the linear resistance of a three dimensional lattice Superconductor model in the London limit London lattice model by Monte Carlo simulation of the vortex loop dynamics. We find excellent finite size scaling at the phase transition. We determine the dynamical exponent $z = 1.51$ for the isotropic London lattice model.

The fluctuation regime in high T_c superconductors (HTCS) is expected to be sufficiently wide that critical fluctuations are observable [1,2]. In particular the conductivity is supposed to scale as $\sigma \propto \xi^{2-d+z}$ [1,2], where ξ is the correlation length and d is the dimension of the system. This scaling relation has been applied in recent experiments on YBCO in zero magnetic field [3]. From which the value $z \approx 2.6$ and $\nu \approx 1.2$ (ν is the correlation length exponent) was extracted. Accordingly an accurate determination of z and ν in models of high T_c superconductors is of great interest. The phenomenology of superconductors is described by the Ginzburg–Landau (GL) model. The model is too complicated to allow all degrees of freedom to be included in calculations. Among the standard approximations of the GL model one can mention: the XY [4,5], Villain [6–8], and the lattice superconductor model in the London limit [9–16].

In the present paper we determine z in the zero field London lattice model (LLM). The exponent z is known to be close to 3/2 in the 3 dimensional XY–model, corresponding to model (E) [17].

It is of interest to know whether the London model in which the spin wave degrees of freedom are integrated out is characterised by the same exponent. Equilibrium properties of the XY and the LLM for $\lambda = \infty$ are known to be the same since they are connected through the Villain duality transformation [6]. However, the dynamical properties might not be the same. It is seen in other systems where the spin degrees of freedom have an effect on the dynamics of the topological defects [18]. However, as we show below, in fact the LLM has $z = 1.5$. This result is reassuring given that the model is used to study the dynamics of vortex systems in the relation to HTCS [19].

Since the magnetic field $H_{mag} = 0$ we can limit our study to the isotropic system. We derive an expression for the resistance R , based on the Nyquist formula [20] for voltage fluctuations. From the Nyquist formula we derive a simple finite size scaling relation for the resistivity at the critical temperature T_c and determine the critical dynamical exponent z .

The LLM describes the vortex loop fluctuations of a bulk superconductor. The model originates from a Ginzburg – Landau description with no amplitude fluctu-

ations and the spin waves integrated out within a Villain approximation. On a cubic lattice a vortex loop consists of four line elements forming a closed loop.

The LLM is defined by the partition function Z on a cubic lattice of side length L using periodic boundary conditions:

$$Z = \text{Tr} \exp[-\beta H] \quad (1)$$

$$H = \sum_{\alpha=1}^3 \sum_{i,j} q_{\alpha i} G_{\alpha}(\mathbf{r}_i - \mathbf{r}_j) q_{\alpha j} \quad (2)$$

where H is the Hamiltonian, the link variables q_{α} represent the vortex line elements. There are three kinds of q_{α} , one for each direction $\mathbf{e}_x, \mathbf{e}_y$ and \mathbf{e}_z . The positions, of q_{α} , are given by r_i . The link variables $q_{\alpha i} \in \{-1, 0, 1\}$ take the values 0 and ± 1 . The sum of q_{α} over a unit cube equals zero. This is achieved by the trial updating algorithm, only to add closed vortex loops to the system. The Greens functions $G_{\alpha}(\mathbf{r})$ [13] are given by:

$$G_z(\mathbf{r}) = \frac{1}{L^3} \sum_{\mathbf{k}} \frac{\left(\kappa^2 + \frac{d^2}{4\lambda_z^2}\right) \pi^2 e^{i \mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)}}{\left(\kappa^2 + \frac{d^2}{4\lambda_x^2}\right) \left(\kappa_x^2 + \kappa_y^2 + \frac{J_z}{J_x} \kappa_z^2 + \frac{d^2}{4\lambda_z^2}\right)}, \quad (3)$$

$$G_x(\mathbf{r}) = G_y(\mathbf{r}) = \frac{1}{L^3} \sum_{\mathbf{k}} \frac{\pi^2 e^{i \mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)}}{\left(\kappa^2 + \kappa_y^2 + \frac{J_z}{J_x} \kappa_z^2 + \frac{d^2}{4\lambda_x^2}\right)}, \quad (4)$$

where \mathbf{k} are the reciprocal lattice vectors, k_x, k_y , and $k_z = 2\pi n/L, n = 0, \dots, L-1$, $\kappa^2 = \kappa_x^2 + \kappa_y^2 + \kappa_z^2$ and $\kappa_x = \sin(k_x/2d)$, d is the side length of the unit cell and is set to $d = 1$. The λ_x and λ_z are the bare magnetic penetration lengths in the x and z directions. The coupling constants J_x and J_z determine the anisotropy of the model and are related to the screening length by $J_z/J_x = \lambda_x^2/\lambda_z^2$. In the work presented in this letter the penetration length is taken to be infinite, $\lambda_x = \lambda_z = \infty$, we further restrict the model to the isotropic case $J_x = J_z = 1$.

We simulate the model defined by eq. 2 by the standard Metropolis Monte Carlo method [21]. The trial move consists of adding a closed vortex loop formed out of 4 link variables q . The loop is placed at a randomly chosen position and with one of the 6 different orientations at random.

The standard test for superconducting coherence of a model superconductor has been to sample the helicity modulus $1/\epsilon$:

$$\frac{1}{\epsilon(k)} = 1 - \frac{8\pi^2}{k^2 T L^3} \langle q_{\alpha k} q_{\alpha - k} \rangle \quad (5)$$

In the limit $k \rightarrow 0$ the phase transition is detected in the following way. For temperatures in the superconducting phase $1/\epsilon \neq 0$ and above the transition $1/\epsilon = 0$

In this letter we use an alternative test for the superconducting transition namely the vanishing of the resistance [11]. The dissipation in a 3 dimensional superconductor is caused by the creation of vortex loops and expanding them out to the system boundary. Alternatively if there is an external magnetic field that gives vortex lines through the system, the movement of these vortex lines will dissipate energy. The linear resistivity is defined by $\rho = E/j$ for $j \rightarrow 0$, where j is the applied supercurrent density and E is the resulting induced electric field. The resistance R is given by the Nyquist formula [20,22]

$$R = \frac{1}{2T} \int_{-\infty}^{+\infty} dt \langle V(t)V(0) \rangle. \quad (6)$$

The integral is evaluated as a sum over discrete time steps, defined as one MC trial move. The voltage $V_x(t)$ is defined by the fluctuation of loops and is calculated by the following procedure. $\dot{N}_{x+}(\dot{N}_{x-})$ denotes the number of accepted trial moves with a vortex-loop oriented in the x -direction as $x+$ ($x-$) for a MC sweep through the lattice. The $+$ and $-$ keep track of whether the vortex-loop is positively or negatively oriented. The voltage $V_x(t)$ at time t , in the x -direction, is $V_x(t) \propto \dot{N}_{x+} - \dot{N}_{x-}$. There are three resistances R_x, R_y and R_z which all are equal in the isotropic case considered here.

We consider now the finite size scaling. In three dimensions $1/\epsilon$ obeys the scaling relation [23,24]

$$L \frac{1}{\epsilon(k = \frac{2\pi}{L})} \approx \text{constant} \text{ at } T = T_c \text{ and } d = 3, \quad (7)$$

A finite size scaling relation for the resistivity, can be derived in the following way. The Josephson relation

$$V \sim \frac{d}{dt} \nabla \phi \quad (8)$$

relates the voltage to the time derivative of the gradient of the phase ϕ of the superconducting order parameter [25]. From eq 8 we conclude that as T_c is approached the voltage scales as $V \sim 1/\tau$ where τ is the dynamical time scale. Dimensional analysis of eq. 6 leads to $R \sim 1/\tau$, where τ is related to the correlation length through $\tau \sim \xi^z$. At T_c the correlation length is cut off by the finite size L of the system and we have

$$R \sim \tau^{-1} \sim \xi^{-z} = L^{-z} \quad (9)$$

In three dimensions we have the following relation for the resistivity, $\rho = RL$. Hence, the following finite size scaling relation for the resistivity:

$$\rho L^{z-1} \approx \text{constant} \text{ at } T = T_c \text{ and } d = 3, \quad (10)$$

The Meptropolis algorithm does not in itself contain any reference to time. One can however show [26] that there is a linear relation between time the scale of Langevin dynamics and Metropolis MC trial moves. The success of this similarity has proven itself in many simulations [10,11].

Now we turn to the results. The analysis is based on the finite size scaling relation eq. 10. The temperature is measured in units of J_x . The determination of z is done by the following minimisation procedure on our Monte-Carlo data. For a given value of z , we form the data curves $\rho(L, T)L^{z-1}$ as a function of temperature. We calculate the average separation S_T and S_ρ between the crossings of these curves. The index T and ρ indicate the respective coordinates. For n curves there will be $\sum_{i=1}^{n-1} i$ crossings. The minimum S indicates the z for which the scaling relation eq. 10 is full filled, and it determines the critical temperature T_c . In figure 1 the functions S_T and S_ρ are plotted versus $z - 1$. The lattice sizes in the figure are $L = 8, 10, 12, 14, 16$. Both functions have a clear minimum, which occurs at nearly the same value $z - 1 = 0.51$. Less well converged data will not have coinciding minima for the S_T and S_ρ functions. We have also tried to exclude some of the lattice sizes in the calculation of S_T and S_ρ but this does not change the result for z , at maximum 3%. Including lattice sizes $L = 4$ and 6 will change the determination of z . Especially $L = 4$ is outside the scaling regime and including both $L = 4$ and 6 would change z to 1.51. The critical temperature is determined as the average intersection at the z that minimised S_T and S_ρ and is found to be $T_c = 5.99$.

One might also note that if the data had not been well converged. The minimum in figure 1 would have been less well pronounced. This is because the scaling exponent $z - 1$ is found to be small. For high temperatures there will always be the trivial scaling as there are no finite size effects in ρ for temperatures far above T_c , and eventually one would find $z = 1$ far above T_c . The inset of figure 1 shows the calculated critical temperature versus the scaling exponent $z - 1$. From the inset we see that a large change of the scaling exponent $z - 1$ only gives a moderate change in T_c . Taken together with the well defined minimum in S_T and S_ρ we infer that the procedure to determine z is stable.

In figure 1b the finite size scaling is shown for $1/\epsilon$ in accordance with eq. 7. The evaluated critical temperature corroborates the result achieved with the resistivity scaling. The critical temperature determined is in good agreement with determinations for the 3 dimensional Villain model [8]. There are no adjustable parameters in this

procedure and we can clearly see there is a small finite size effect, as the the curves for larger lattices intersect at slightly lower temperatures. One might also note that as the scaling relation for $1/\epsilon$ works it indicates that the statistic scaling exponents are the same as for the 3 dimensional XY -model.

In figure 2 the resistance scaling is shown for the z that minimised the spread in figure 1. The data shows a very good splay at T_c and eq. 10 is obeyed to high precision. The inset shows the resistivity as a function of temperature. From figure 2 it is evident that there is a small finite size effect. The curves for larger lattices cross at higher temperatures. The effect is small and T_c will have its upper bound given from the $1/\epsilon$ scaling shown in figure 1b. From the inset in figure 1a an approximate value for z would be 1.5.

We have used the Nyquist relation to determine T_c directly from the vanishing resistivity. From the size scaling near T_c we determine the dynamical critical exponent z to be $z = 1.51 \pm 0.03$. This result is interesting since it is equivalent to superdiffusive behaviour. Most models have subdiffusive behaviour, i.e. $z > 2$ [27]. It is also worth to emphasis that the result establish that the 3d XY -model and the 3d London lattice model has the same dynamical critical behaviour not only the same equilibrium exponents. It is interesting to compare our result to a recent work by Wengel and Young [16] a study of the Lattice superconductor in the limit $\lambda = 0$ was presented. In this limit of the model they find $z = 3$. The difference between our result and their result is consistent with the fact that LLM for $\lambda < \infty$ is not equivalent to the XY -model.

We thank Petter Minnhagen, Peter Olsson and Steve Teitel for useful discussions. H. W. was supported by grants from Carl Trygger and from the Kempe foundations. H. J. J. was supported by the British EPSRC grant no. Gr/J 36952. The authors also acknowledge C. Sire for the the reference to Majumbar.

-
- [1] D. S. Fisher, M. P. A. Fisher, and D. A. Huse, Phys. Rev. B **43**, 130 (1991).
 - [2] A. Dorsey, M. Huang, and M. P. A. Fisher, Phys. Rev. B **45**, 523 (1992).
 - [3] James C. Booth, Dong-Ho Wu, S. Qadri, E. Skelton, M. S. Osofsky, Alberto Pique, and Steven M. Anlage, Unpublished, 1996.
 - [4] H. Weber and H. J. Jensen, Phys. Rev. B **44**, 454 (1991).
 - [5] Y. -H. Li and S. Teitel, Phys. Rev. Lett. **66**, 3301 (1991); Phys. Rev. B **47**, 359 (1993); Phys. Rev. B **49**, 4136 (1994).
 - [6] J. Villain, J. de Phys. **36**, 581 (1975).
 - [7] W. Janke and K. Nather, Phys. Rev. B **48**, 7419 (1993).

- [8] W. Janke and T. Matsui, Phys. Rev. B **42**, 10673 (1990).
- [9] J. -R. Lee and S. Teitel, Phys. Rev. Lett. **64**, 1483 (1990); Phys. Rev. B **46**, 3247 (1992);
- [10] J. -R. Lee and S. Teitel, Phys. Rev. B **50**, 3149 (1994).
- [11] M. Wallin and H. Weber, Phys. Rev. B **51**, 6163 (1995); H. Weber, M. Wallin and H. J. Jensen, Phys. Rev. B **53**, 8566 (1996).
- [12] S. E. Korshunov, Europhys. Lett. **11**, 757 (1990).
- [13] G. Carneiro, R. Cavalcanti, and A. Gartner, Europhys. Lett. **17**, 449 (1992), Phys. Rev. B **47**, 5263 (1993),
- [14] T. Chen and S. Teitel, Phys. Rev. Lett. **74**, 2792 (1995).
- [15] S. Ryu and D. Stroud, unpublished (1996).
- [16] C. Wengel and A. P. Young, unpublished, cond-mat/9605087.
- [17] P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).
- [18] K. Damle, S. N. Majumbar and S. Sacdev, unpublished, cond-mat/9511058.
- [19] E. A. Jagla and C. A. Balseiro, Phys. Rev. B **53**, R538 (1996), Phys. Rev. B **53**, 15305 (1996).
- [20] F. Reif, *Fundamentals of statistical and thermal physics*, McGraw-Hill (1965).
- [21] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).
- [22] A.P. Young, The Vortex Glass, Proceedings of the Ray Orbach Inauguration Symposium, World Scientific (1993).
- [23] M. -C. Cha, M. P. A. Fisher, S. M. Girvin, M. Wallin and A. P. Young, Phys. Rev. B **44**, 6883 (1991).
- [24] Y. -H. Li and S. Teitel, Phys. Rev. B **40**, 9122 (1989).
- [25] M. Tinkham, *Introduction to Superconductivity*, McGraw-Hill (1975).
- [26] P. Meakin, H. Metiu, R. G. Petschek, and D. J. Scalapino, J. Chem. Phys. **79**, 1948 (1983).
- [27] S. K. Ma, *Modern Theory of Critical Phenomena*, Benjamin-Cummings (1976).

FIG. 1. Monte Carlo results for the LLM. Shown in figure a are results for the scaling relation eq. 10. The functions S_ρ (dashed curve) and S_T (solid curve) are drawn as function of the dynamical exponent z . The lattice sizes employed in the determination are $L = 8, 10, 12, 14$ and 16 . The minimum occurs at $z = 1.51$. The critical temperature of the system is determined to $T_c = 5.99$. The inset shows the determined T_c as a function of z . In figure b the results for the scaling relation eq. 7 are shown. Lattice sizes L are $4 = \text{stars}$, $6 = \text{open circles}$, $8 = \text{filled circles}$, $10 = \text{open squares}$, $12 = \text{filled squares}$, $14 = \text{triangles}$ and $16 = \text{plusses}$. One can clearly see the curves for larger lattices intersect at lower temperatures.

FIG. 2. Monte Carlo results for the scaled resistivity. The function $\rho(T)L^{z-1}$ is plotted against temperature. The dynamical exponent is determined from figure 1a $z = 1.51$. Lattice sizes L are $4 = \text{stars}$, $6 = \text{open circles}$, $8 = \text{filled circles}$, $10 = \text{open squares}$, $12 = \text{filled squares}$, $14 = \text{triangles}$ and $16 = \text{plusses}$. There is a finite size effect present, intersections for the larger lattices take place at a slightly higher temperature. The inset shows ρ as a function of T .

Weber Jensen Fig 1a





