Monte Carlo Calculation of the Linear Resistance of a Three Dimensional Lattice superconductor Model in the London Limit

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We have studied the linear resistance of a three dimensional lattice superconductor model in the London limit 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. [S0031-9007(97)02775-0]

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The fluctuation regime in high T_c superconductors (HTSC) 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 values $z \approx 2.6$ and $\nu \approx 1.2$ (ν is the correlation length exponent) were 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 are the XY [4,5], Villain [6–8], and the lattice superconductor model in the London limit [9–15].

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 three dimensional XY model, corresponding to model (E) [16], the symmetric planar magnet in zero external magnetic field.

It is of interest to know whether the London model in which the spin wave degrees of freedom are integrated out is characterized 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. This is seen in other systems where the spin degrees of freedom have an effect on the dynamics of the topological defects [17]. 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 HTSC [18].

Since the magnetic field $H_{\mathrm{mag}} = 0$ we can limit our study to the isotropic system. We derive an expression for the resistance R, based on the Nyquist formula [19] 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 fluctuations 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,

$$Z = \mathrm{Tr}\,\exp[-\beta H], \tag{1}$$

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

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 $q_{\alpha i} \in \{-1, 0, 1\}$. The sum of q_α over a unit cube equals zero. This is achieved by the trial updating algorithm, which only adds closed vortex loops to the system. The Green's functions $G_\alpha(\mathbf{r})$ [13] are given by

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

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

where $\mathbf{k}$ are the reciprocal lattice vectors, k_x, k_y, and $k_z = 2\pi n/L, n = 0, \ldots, L-1$, $\kappa^2 = \kappa_x^2 + \kappa_y^2 + \kappa_z^2$ 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 $J_x = J_z = 1$.

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We simulate the model defined by Eq. (2) by the standard Metropolis Monte Carlo (MC) method [20]. 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 $1/\epsilon$,

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

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 three 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 [19,21]

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

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 x direction refers to the vector normal to the vortex loop plane. 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 $V_x(t) \propto \dot{N}_{x+} - \dot{N}_{x-}$. As a loop is accepted this implies the expansion of the link elements over an elementary square. In the corresponding XY model this is associated with a phase slip, by the Josephson relation [22], and hence the voltage $V_x(t)$. The resistances R_x, R_y, and R_z 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]

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

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 [22]. 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 relation $\rho = RL$ for the resistivity. Hence, the following finite size scaling relation for the resistivity:

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

The Meptropolis algorithm does not in itself contain any reference to time. One can, however, show [25] that there is a linear relation between the time scale of Langevin dynamics and Metropolis MC trial moves. The success of this similarity has proven itself in many simulations [10,11]. This argument indicates that our MC dynamics is a faithful representation of the Langevin dynamics of a gas of vortex loops. We cannot be certain about the relationship between the dynamics of our model and the dynamics of a real superconductor as represented, e.g., by the time dependent Ginzburg Landau equations (TDGLE). The TDGLE contains amplitude and linear phase fluctuations. Both types of fluctuations are absent in the London model. However, the dynamical equivalence we have established between the 3D XY model and the London model shows that the absence of linear phase fluctuations are inessential. It is therefore possible that the considered MC dynamics of the London model is equivalent to the vortex dynamics of a real superconductor.

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 minimization procedure on our Monte Carlo data. For a specific value of z, we form the data curves $\rho(L,T)L^{z-1}$ as a function of T. Depending on the choice of z the crossings, of these curves, will be more or less well gathered. Their average separation along the T axis (or ρ axis) will be denoted $S_T(z)$ [or $S_\rho(z)$]. The common minima of S_T (or S_ρ) determines the z for which the scaling relation Eq. (10) is fulfilled. In Fig. 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 1.49. We identify T_c as the average value of T for which the set of $\rho(L,T)L^{z-1}$ curves cross each other and S_T has its minimum.

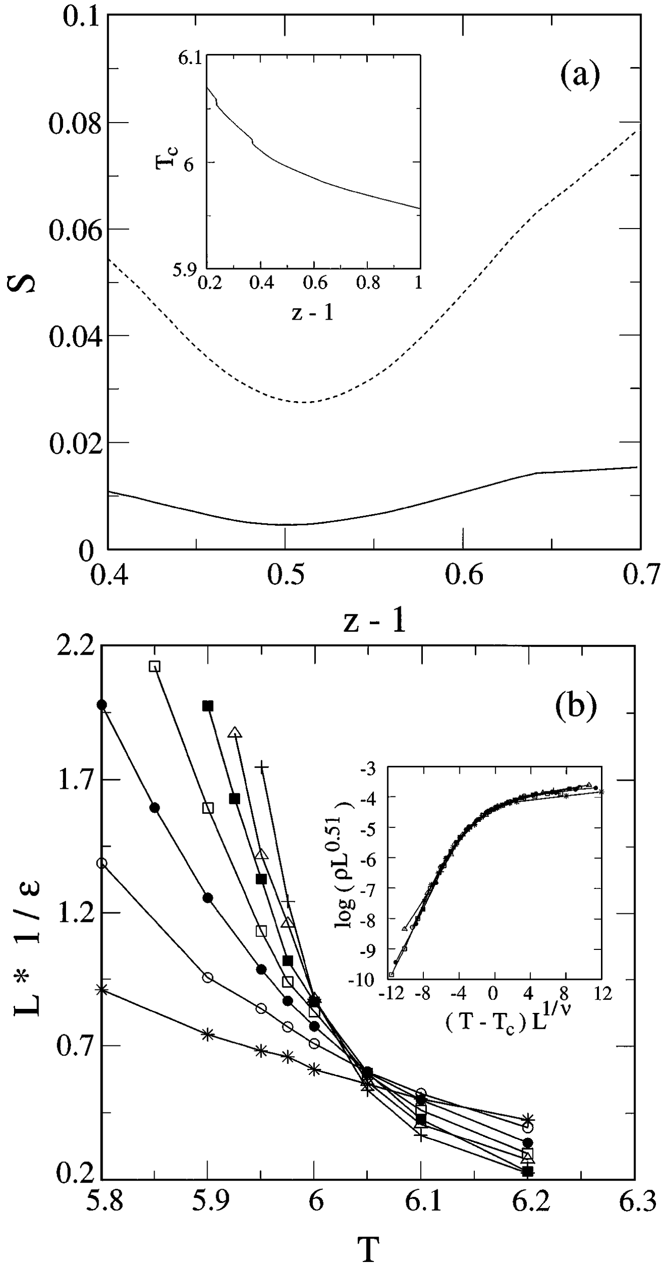

FIG. 1. Monte Carlo results for the LLM. Shown in (a) are results for the scaling relation Eq. (10). The functions S_ρ (dashed curve) and S_T (solid curve) are drawn as a function of the dynamical exponent z. The lattice sizes employed in the determination are $L = 8, 10, 12, 14$, and 16. The minimum 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 (b) the results for the scaling relation Eq. (7) are shown. Lattice sizes L are 4 = stars, 6 = open circles, 8 = filled circles, 10 = open squares, 12 = filled squares, 14 = triangles, and 16 = plusses. One can clearly see that the curves for larger lattices intersect at lower temperatures. The inset shows ρL^{z-1} as a function of $(T - T_c)^{1/\nu}$, $\nu = 0.669$ for the static 3D XY model.

One might also note that if the data had not been well converged, the minimum in Fig. 1(a) 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. We check now how strongly T_c depends on the chosen value of $z - 1$. We plot in the inset of Fig. 1(a) the value of T_c determined (like we did above) as the average value of the abscissa of the crossings of the $\rho(L,T)L^{z-1}$ versus T curves for different values of $z - 1$. We see that a small change in T_c corresponds to a large change in $z - 1$. Taken together with the well defined minimum in S_T and S_ρ we infer that the procedure to determine z is stable.

In Fig. 1(b) 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 three 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 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 static scaling exponents are the same as for the three dimensional XY model. This is also corroborated by hyperscaling of ρL^{z-1} versus $(T - T_c)^{1/\nu}$, which is shown in the inset of Fig. 1(b). Here $\nu = 0.669$ [26] is the static exponent from the 3D XY model, and for z and T_c we have used the values determined by the procedure above.

In Fig. 2 the resistance scaling is shown for the z that minimized the spread in Fig. 1. The data show 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 Fig. 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 Fig. 1(b). From the inset in Fig. 1(a) 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 behavior. Most models have subdiffusive behavior, i.e., $z > 2$ [27]. It is also worth emphasizing that the results establish that the Dd XY model and the 3D London lattice model have the same dynamical critical behavior, not only the same equilibrium exponents. It is interesting to compare our result to a work by Lee and Stroud [28] where a study of the 3D resistively shunted junction (RSJ) model with Langevin dynamicsis described. They study the current-voltage characteristics and from it deduce $z = 1.5 \pm 0.5$.

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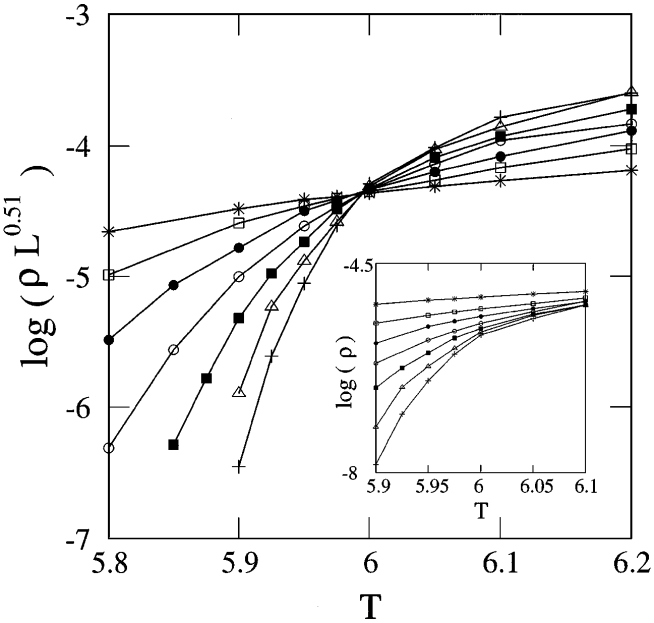

FIG. 2. Monte Carlo results for the scaled resistivity. The function $\rho(T)L^{z-1}$ is plotted against temperature. The dynamical exponent is determined from Fig. 1(a) $z = 1.51$. Lattice sizes L are 4 = stars, 6 = open circles, 8 = filled circles, 10 = open squares, 12 = filled squares, 14 = triangles, and 16 = 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.

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