Disorder-induced first-order transition in superconducting films

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Strong disorder in the two-dimensional XY model is shown to favor the first-order phase transition with nonuniversal properties due to reduction of the effective temperature for short-scale fluctuations. The results seem to be of relevance for high-T_c superconducting films.

In recent experiments on c-axis-oriented $YBa_2Cu_3O_7$ thin films[1] the behavior of the inverse penetration depth Λ^{-1} in the vicinity of the phase transition was investigated. The authors of Ref. 1 interpreted their data as proof of a very sharp but continuous decrease of Λ^{-1}. Such an interpretation is, to some extent, in contradiction with existing theoretical understanding of the properties of such systems. As is well known in two-dimensional systems with continuous degeneracy, there is no way to prevent the Berezinskii-Kosterlitz-Thouless unbinding of vortex pairs from happening at still finite values of the helicity modulus (or, equivalently, Λ^{-1}). The phase transition certainly can take place due to some other mechanism,[2–7] but only at lower temperatures than the expected vortex pair unbinding, so the jump in that case would be even larger than the universal value. In this context the results of Ref. 1 can be also interpreted as evidence for the nonuniversal jump in Λ^{-1} slightly broadened by finite-frequency or inhomogeneity effects.

As high-T_c superconducting films are known to possess a somewhat irregular structure, it seems reasonable to make an attempt to relate the nonuniversal jump to disorder. The theoretical description of various two-dimensional superconducting systems is usually done with the help of some kind of XY model, which has the same continuous degeneracy of the ground state. During recent years most attention on the problem of disorder in XY models was concentrated on so-called positional disorder, corresponding to the inclusion of a random phase shift on each of the bonds of the lattice.[8,9] Such disorder appears only in the presence of the magnetic field. The disorder in the coupling constant that proves to be irrelevant in terms of the renormalization group[8] was considered to be of no particular interest. Since the renormalization arguments are applicable only for small disorder, there always remains a possibility that strong disorder may change the type of the transition.

In the present paper the influence of strong disorder on properties of the phase transition in two-dimensional superconducting systems is investigated with the help of the XY model with a random coupling constant. In the framework of the replica representation we study how strong disorder changes the form of the effective nearest-neighbor interaction and show that the tendency towards a first-order transition is developed.

The idea that in the XY model a first-order transition induced by anharmonicities can occur was already put forward in 1973.[2] Later it was confirmed by computer simulations that by changing in some particular way the interactions in the XY model it is possible to obtain a discontinuous phase transition with the jump in the vortex density.[3–5]

One of the ways to do this consists in substitution of the pure cosine interaction,

$$V(\nabla\phi) = J[1-\cos(\nabla\phi)], \quad \nabla\phi \equiv \phi_j - \phi_{j'}$$

with some other periodic function of phase difference that favors the short-scale fluctuations. This is achieved when a ratio of

$$\Delta V = V(\pi) - V(0)$$

to

$$V''(0) \equiv \left.\frac{\partial^2 V}{\partial \phi^2}\right|_{\phi=0}$$

is much lower than for $V_0(\phi) = 1-\cos\phi$.[4]

For such an interaction the effective temperature for the long-wavelength fluctuations (spin waves and vortices) turns out to be much higher than for the short-scale fluctuations (rotations of separate spins by large angles). It makes possible the disordering induced by local fluctuations to take place at temperatures at which the vortex-vortex interaction is still stronger than at the point of the Berezinskii-Kosterlitz-Thouless transition, thus making the helicity-modulus jump nonuniversal. In Monte Carlo simulations[4,5] the interaction function of the form

$$V(\phi) = 2J[1-\cos^{2p^2}(\phi/2)]$$

was used, which for $p \gg 1$ has a very narrow well in the vicinity of $\phi = 0$ with $V''(0) = Jp^2$ and an almost flat plateau for other values of ϕ with $\Delta V = 2J$. The transition was shown to change its order at $p^2 \sim 10$.[5]

Another possibility of causing the phase transition in the XY model to become first order consists in increasing the fugacities of the vortices until the vortex pairs start overlapping at low enough temperatures when they are supposed to be tightly bound. It was shown both in Monte Carlo simulations[3] and analytically (with the help of the generalization of the Kosterlitz renormalization equations[6,7]) that this also causes the transition to become first order. Both methods are compatible with each other because for the interaction function with

$\Delta V \ll V''(0)$ the fugacity of the vortices is strongly increased.

In the following we show that the same tendency towards first-order phase transition develops in the case of a strong disorder in the coupling constant. Let us start from the Hamiltonian:

$$H = \sum_{j,j'} J_{jj'}[1 - \cos(\phi_j - \phi_{j'})], \tag{1}$$

where the summation is performed over pairs of nearest neighbors on some regular two-dimensional lattice. Factor $\beta \equiv 1/(k_B T)$ is assumed to be included into the definition of $J_{jj'}$. Following standard procedure[10] n replicas of (1) numbered by greek indices $\alpha = 1, \ldots, n$ can be introduced. After that the partition function should be averaged over disorder. We use a very simple model in which each coupling constant can have only two different values: J_0 with probability c and J_1 with probability $1-c$. So the case of strong disorder corresponds to $J_0 \ll J_1$. We do not discuss the case of $J_0 = 0$ in order to avoid the possibility of a geometrical percolative transition.

Taking the average over disorder leads then to the Hamiltonian for the replicated variables ϕ^α, which can be written as

$$H = \sum_{j,j'} W_0(\Sigma\{\phi\}), \tag{2}$$

where

$$W_0(x) = -\ln[c\exp(-J_0 x) + (1-c)\exp(-J_1 x)],$$
$$\Sigma\{\phi\} = \sum_\alpha V_0(\nabla\phi^\alpha), \tag{3}$$
$$\nabla\phi^\alpha \equiv \phi_j^\alpha - \phi_{j'}^\alpha, \quad V_0(\phi) = 1 - \cos\phi.$$

The ground state of (2) corresponds to all ϕ_j^α's in the same replica being equal to each other. The expansion to the lowest order in fluctuations gives

$$H = \sum_\alpha \sum_{j,j'} \frac{J_{\text{eff}}}{2}(\nabla\phi^\alpha)^2, \tag{4}$$

where $J_{\text{eff}} = cJ_0 + (1-c)J_1$ can be considered the effective-coupling constant.

Hamiltonian (2), just like Hamiltonian (1), allows for the introduction of vortex solutions. From the form of Eq. (4) it is evident that only the interaction of vortices belonging to the same replica is logarithmic, but in the case of different replicas it is short ranged. So in the renormalization the interaction of vortices in different replicas turns out to be irrelevant,[8] that being the reason for the absence of interest in coupling constant disorder. Now we intend to study more attentively the form of the effective Hamiltonian for fluctuations in one replica, and later we will also add to it the influence of interaction between replicas.

If we completely suppress fluctuations in all the replicas but one we obtain the Hamiltonian of the ordinary XY model with the interaction function:

$$V(\phi) = W_0[V_0(\phi)], \tag{5}$$

which for the case of strong disorder ($J_0 \ll J_1$) proves to possess the very same features that are needed to obtain the first-order transition. For the case of low temperatures ($J_1 \gg 1$) comparison of $V''(0) \equiv J_{\text{eff}}$ with $\Delta V \approx 2J_0$ shows that the presence of disorder strongly decreases ΔV in comparison with $V''(0)$. For any value of $V''(0)$, ΔV can be made arbitrarily small by the proper choice of J_0. Thus the short-scale fluctuations are strongly favored and can be made sufficiently large to induce the first-order transition.

Such an approach would be exact if the fluctuations in the coupling constant were not quenched but thermodynamical so that there would be only one replica to consider. In the case of a quenched disorder the interaction with the other replicas should also be taken into account. As we have seen, the interaction of large-scale fluctuations (vortices) in different replicas is not very important, so we shall calculate the contribution from the fluctuations in all the other replicas to the effective Hamiltonian of one particular replica assuming these fluctuations to be short ranged. In order to do this we expand Eq. (3) to the lowest order in fluctuations of ϕ^α ($\alpha = 2, \ldots, n$) for an arbitrary configuration of the field ϕ^1, obtaining thus

$$H = \sum_{j,j'} \left\{ W_0[V_0(\nabla\phi)] + \frac{1}{2}\sum_{\alpha=2}^{n} \left.\frac{dW_0(x)}{dx}\right|_{x=V_0(\nabla\phi)} (\nabla\phi^\alpha)^2 \right\}, \tag{6}$$

where we have omitted index 1 in ϕ^1.

Now the Gaussian fluctuations in all the replicas but the first can be integrated out, obtaining thus the correction to the interaction function (5), which it would be convenient to express in terms of the correction to $W_0(x)$:

$$W(x) = W_0(x) + \delta W(x), \quad \delta W(x) = -\frac{1}{2}\ln\frac{dW_0}{dx}, \tag{7}$$

where we have already put n equal to zero. For $W_0(x)$ of the form (3), $\delta W(x)$ can be written as

$$\delta W(x) = -\frac{1}{2}\ln\left\{ J_0 + \frac{(J_1 - J_0)(1-c)}{1 - c + c\exp[(J_1 - J_0)x]} \right\}. \tag{8}$$

It can be seen that the correction (8) works in the opposite direction, increasing the value of

$$\Delta V \equiv W(2) - W(0)$$

so that for the fixed value of

$$V''(0) = \left.\frac{dW}{dx}\right|_{x=0}$$

it becomes impossible to make ΔV arbitrarily low.

However, the higher-order corrections partly reduce the undesirable increase of ΔV. If instead of calculating the contribution from the Gaussian fluctuations in $(n-1)$ replicas with the help of the unrenormalized interaction function $W_0(x)$ we assume that they are determined by the renormalized one $W(x)$, the self-consistent equation of the form

$$W(x) = W_0(x) - \frac{1}{2}\ln\frac{dW}{dx} \tag{9}$$

would be obtained; this accounts for the influence of the interreplica interaction on $W(x)$ in a more sophisticated way than Eq. (7). For $W_0(x)$ of the form (3) the solution of (9) can be written as

$$W(x) = \frac{1}{2}\ln\frac{I(x)}{J_1 - J_0},$$

$$I(x) = \int_0^{\exp(J_1-J_0)x} dy \frac{y^b}{(1-c+cy)^2}, \tag{10}$$

$$b = \frac{J_1 + J_0}{J_1 - J_0}.$$

In the limiting case of $J_0 \ll 1 \ll J_1$, Eq. (10) gives

$$V''(0) \approx \frac{c^2}{\ln\frac{1}{1-c} - c} J_1, \tag{11}$$

$$\Delta V \approx \frac{1}{2}\left(1 + \frac{2J_1 + \ln c}{\ln\frac{1}{1-c} - c}\right). \tag{12}$$

Comparison of Eqs. (10)–(12) with the results of Ref. 5 shows that for c in the intermediate range between $\frac{1}{2}$ and 1 our model is on the very edge of changing the order of the phase transition. As the effective interaction function $V(\phi) = W[V_0(\phi)]$ corresponds only to some approximate description of the system, it is impossible to make a definite conclusion as to whether such a change will really occur, but it is very probable.

Thus our calculation has given some support to the idea that the type of the phase transition in thin superconducting films may be changed due to the influence of strong disorder. Certainly the considered model is very simple and cannot be applied to the detailed description of such films or direct comparison with experimental results. Nonetheless, it definitely demonstrates the strong tendency towards a first-order phase transition (with the nonuniversal jump of the inverse penetration depth Λ^{-1}) that is induced by the randomness in the coupling constant.

A more appropriate model for the granular superconducting film should incorporate disorder not only in the strength of the coupling, but also in the lattice structure. If this other kind of disorder would enhance the same tendency, our interpretation of the results of the experiments on $YBa_2Cu_3O_7$ thin films[1] would become more convincing. So the problem is still in need of further investigation.

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