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Thermal phase transition in two-dimensional disordered superconductors

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Abstract – Weakly disordered two-dimensional superconductors undergo a Kosterlitz-Thouless (KT) transition, where at a critical temperature vortices proliferate through the system and destroy the superconducting (SC) order. On the other hand, it was suggested that for large disorder the system separates into regions of high SC order, and it is the percolation of coherence between these regions that is lost at the critical temperature. Here we demonstrate that both these descriptions can be applied, suggesting that they are the dual of each other. A vortex causes loss of local correlations, and thus the loss of percolation of correlations is concomitant with percolation of vortices on the dual lattice, in the perpendicular direction, *i.e.* the KT transition.

Introduction. – The interplay of disorder and superconductivity has been a subject of research from the early days of BCS theory [1], when Anderson has demonstrated that weak disorder does not affect the BCS critical temperature [2]. It was later argued that superconductivity indeed persists even when the single-particle states are localized [3], but eventually, with strong enough disorder, superconductivity is destroyed. Thus, the critical temperature is reduced with increasing disorder, until it is suppressed all the way to zero for large enough disorder, indicating a zero-temperature transition from a superconducting (SC) to an insulating phase. The situation is even more intriguing in two dimensions, where, even without disorder, there could be no long-range SC order at any finite temperature T due to the Mermin-Wagner theorem [4]. Nevertheless, one expects a finite-temperature Kosterlitz-Thouless (KT) transition [5] between a phase with power-law decaying correlations to a phase with exponentially decaying correlations. This transition is driven by the unbinding and proliferation of vortex-anti vortex pairs, which destroy the SC order. The effect of disorder on the KT transition has become even more relevant since the experimental observation of superconductor-insulator transition in thin disordered films, about two decades ago [6,7]. Weak disorder should not affect the transition, according to the Harris criterion [8]. In the presence of strong disorder, however, it has been established theoretically [9–12] and observed experimentally [13,14] that the SC order parameter fluctuates strongly across the sample, creating "SC islands", where the SC order is high, surrounded by areas of weaker SC correlations. Thus, with increasing temperature the coherence between neighboring SC islands is quenched, until percolation of coherence from one side of the sample to the other is lost, leading to the loss of global SC order [15,16]. This description predicts that local SC order may persists even when global SC order is lost, consistent with recent experiments [17–19]. This scenario is very similar to the description of granular systems [20], where two grains were considered connected if their effective Josephson coupling was larger than temperature. Thus, as temperature increases, grains become disconnected and percolation is lost. Such a theory was very successful in describing the resistance and specific heat of granular systems.

It is not clear if these two different descriptions, the KT description and the percolation one, describe different transitions, or they are two alternative descriptions of the the same transition. In this letter we study, starting from a microscopic model, the thermal phase transition from a SC to a normal state in amorphously disordered two-dimensional superconductors. In particular we address the question of relevance of these two scenarios to describe this transition.

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Model and method. – We begin with the negative-U Hubbard model,

$$\mathcal{H} = -\sum_{\langle i,j\rangle,\sigma} t_{ij} C^\dagger_{i\sigma} C_{j\sigma} + U \sum_i C^\dagger_{i\uparrow} C^\dagger_{i\downarrow} C_{i\downarrow} C_{i\uparrow} + \sum_{i,\sigma} (V_i - \mu)\, C^\dagger_{i\sigma} C_{i\sigma}, \quad (1)$$

where $\langle i,j\rangle$ indicates a sum over nearest neighbors, $C^\dagger_{i\sigma}$ creates a spin-σ electron at site i, t_{ij} is the hopping integral, taken to be the unit of energy in the following, and $U<0$ is the on-site attractive potential. The site-specific disorder V_i is taken from a uniform distribution of width $2W$ such that $V_i \in [-W, W]$, but for each realization we ensure that $\sum_i V_i = 0$, and the chemical potential μ determines the average density n. The choice of the Hubbard model is because it can lead, depending on parameters, to a BCS transition, to a KT transition or to a percolation transition, and thus it is general enough not to limit a priori the possible transitions, unlike, *e.g.* the XY model, which is known to give rise to a KT transition [5] and may bias the results towards this particular transition.

In order to consider SC fluctuations, crucial for the description of the transition, we employ a method that takes into account thermal fluctuations, but ignores the quantum ones [16,21]. In short, applying a Hubbard-Stratonovic transformation to the Hubbard Hamiltonian (1), with a local complex Hubbard-Stratonovic field, Δ_i, and ignoring the temporal dependence of these fields (quantum fluctuations), the partition function becomes

$$Z = \mathrm{Tr}[e^{-\beta\mathcal{H}}] = \int \mathcal{D}(\{\Delta_i, \Delta_i^*\}) \mathrm{Tr}_f[e^{-\beta\mathcal{H}_{BdG}(\{\Delta_i\})}],$$

with the Bogoliubov-de Gennes Hamiltonian [22] $\mathcal{H}_{BdG}(\{\Delta_i\})$ given by

$$\mathcal{H}_{BdG} = -\sum_{\langle i,j\rangle,\sigma} t_{ij} C^\dagger_{i\sigma} C_{j\sigma} + \sum_{i\sigma} (V_i - \mu + U_i)\, C^\dagger_{i\sigma} C_{i\sigma} + \sum_i \left(\Delta_i C^\dagger_{i\uparrow} C^\dagger_{i\downarrow} + \Delta_i^* C_{i\downarrow} C_{i\uparrow}\right).$$

Here $U_i = \frac{U}{2}\sum_\sigma \langle C^\dagger_{i\sigma} C_{i\sigma}\rangle_{MF}$ is the (self-consistent) Hartree-Fock term and Tr_f traces the fermionic degrees of freedom over the single-body Hamiltonian $\mathcal{H}_{BdG}$ and can be evaluated exactly using its eigenvalues. Instead of diagonalizing the Hamiltonian, one can use a Chebyshev polynomial expansion [23], which makes the calculation less time consuming. The integral over the fields $\{\Delta_i, \Delta_i^*\}$ can then be calculated using the (classical) Metropolis Monte Carlo (MC) technique [24]. One should note that, unlike the usual BdG approach, here Δ_i are auxiliary fields, and except at zero temperature where the saddle point evaluation of the partition function gives rise to the BdG solution, they are generally different from the local SC order parameter $\langle C_{i\downarrow} C_{i\uparrow}\rangle$.

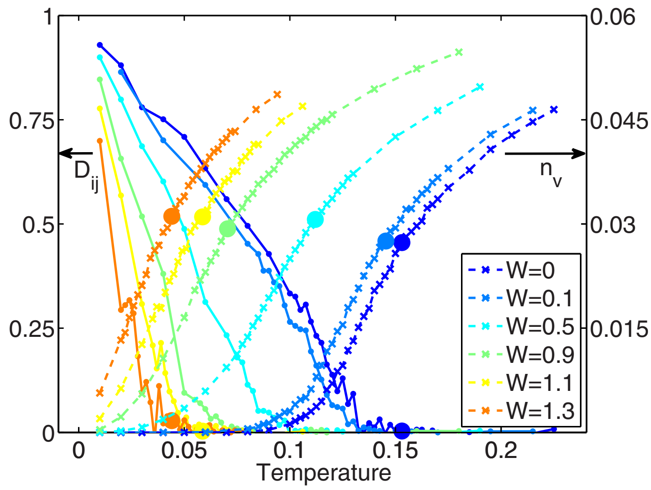


Fig. 1: The edge-to-edge phase correlation D_{ij} (left axis) and the vortex density n_v (right axis) as a function of temperature, for different values of disorder for 18×18 system, and $U=-4$, and values of disorder depicted in the legend. With increasing disorder T_c, where bulk coherence is lost and vortices start to proliferate, shifts to lower values, but the curves still look similar. The circles denote the percolation temperature T_p (see text).

This procedure allows the calculation of any ensemble-averaged quantity. We first calculate the average correlation function $D_{ij} \equiv \langle\cos(\theta_i - \theta_j)\rangle$, where θ_i is the phase of the SC order parameter $\langle C_{i\downarrow} C_{i\uparrow}\rangle$, and i and j are two sites, either on the opposite edges of the sample or nearest neighbors. In principle, a correct measure of SC order is the *off-diagonal long-range order* (ODLRO) [25], $\langle C^\dagger_{i\downarrow} C^\dagger_{i\uparrow} C_{j\uparrow} C_{j\downarrow}\rangle$. By considering correlation between fermion pairs $\langle C^\dagger_{i\downarrow} C^\dagger_{i\uparrow}\rangle$ and $\langle C_{j\uparrow} C_{j\downarrow}\rangle$, D_{ij} approximates the ODLRO and hence the decay of the edge-to-edge D_{ij} to zero signals the loss of bulk SC order in the system. We have confirmed numerically that D_{ij} is a good estimate of ODLRO, while being much easier to compute.

Results: KT transition at finite disorder. – We present results for edge-to-edge D_{ij} in fig. 1. As can be seen in the figure, the coherence is suppressed with increasing temperature, towards zero. Increasing disorder suppresses the critical temperature T_c, as expected. Except for the change in T_c, the decay of correlations at finite disorder looks very similar to the zero-disorder case, expected to be described by the KT transition.

In order to quantify this observation further, we calculate the sample-averaged vortex (and anti-vortex) density, n_v. The local vortex density for a single snapshot during the MC procedure is determined by the clockwise integration of the phase of the SC order parameter around a single plaquette. The value of this integral can assume only integer multiples of 2π, indicating the existence of vortices ($n>0$), anti-vortices ($n<0$), or no vorticity ($n=0$). In fig. 1 we also plot n_v as a function of temperature. As can clearly seen, the loss of global phase coherence occurs

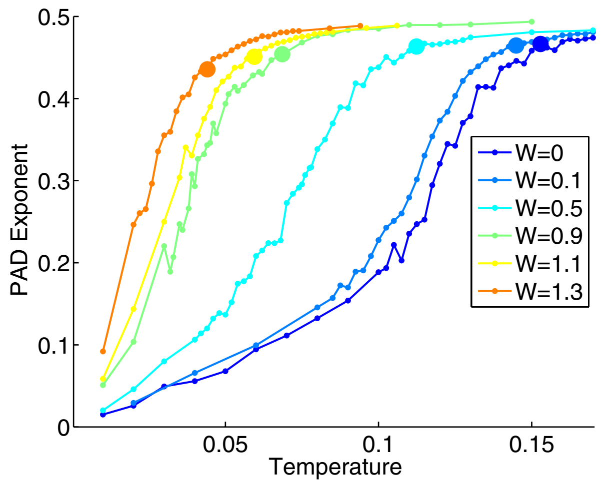


Fig. 2: The PAD exponent [26] α for $U=-4$, 18×18 system for different values of disorder, exhibiting an abrupt change, signalling the transition. Large dots correspond to T_p from the percolation picture (see text).

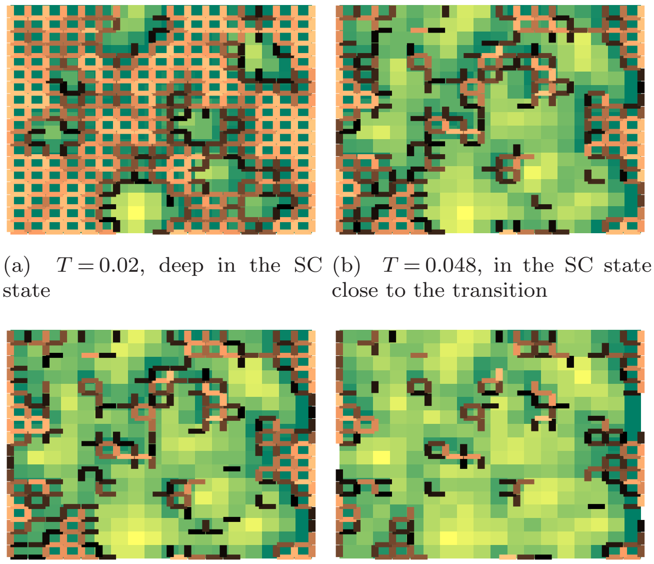
when vortices start to proliferate, for *all values of disorder*, indicating a KT-type transition.

Unfortunately, due to the expected slow decay of correlations near the KT transition, a full finite-size scaling analysis is outside the scope of this paper. In order to further identify the KT characteristics of the transition, we adopt a particularly elegant analysis proposed by Polkovnikov, Altman and Demler [26], and used in experimental analysis by Hadzibabic *et al.* [27]. The idea is to perform the double sum over all pairwise correlations D_{ij}, up to the system size L,

$$A(L,T)\equiv\frac{1}{L^2}\sum_{i=1}^{L}\sum_{j=1}^{L}D_{ij}^2(T)\sim L^{-2\alpha(T)}, \qquad (2)$$

where the second relation defines the exponent α. As $T\to0$ we expect $D_{ij}\to1$ meaning that $A(L,T\to0)=1$ and therefore $\alpha(T\to0)=0$. In the opposite limit, when $T>T_c$ then D_{ij} decays exponentially with the distance $|i-j|$, leading to $A(L,T\geqslant T_c)\to L^{-1}$ and $\alpha\to0.5$. At the KT transition (see [26]), a universal jump from $\alpha=0.25$ to $\alpha=0.5$ is expected.

Figure 2 depicts our results for the PAD exponent α as function of temperature, for different values of disorder. All the curves (except for the highest disorder, probably already on the insulating side) exhibit a very similar behavior —a moderate rise from $\alpha=0$ to $\alpha\simeq0.25$ and then a rather abrupt rise towards $\alpha\simeq0.45$ followed by a a more gradual increase towards $\alpha=0.5$, demonstrating a change from power-law decay of correlations to exponentially decaying correlations, again consistent with the KT description. We attribute the smoothing of the jump in the value of the exponent to the finite size of our system, as the coherence length ξ_0, which is approximately given by $\hbar v_F/\Delta$, where v_F is the Fermi energy and Δ the SC gap, is not much smaller than the system size (about a factor of 2 or 3). The fact that the same behavior is observed at zero disorder, where the KT description is indeed expected to hold, supports this explanation.



(a) $T=0.02$, deep in the SC state
(b) $T=0.048$, in the SC state close to the transition
(c) $T=0.052$ insulating state, just crossed the transition
(d) $T=0.074$ deep in the insulating state

Fig. 3: Percolation transition for a 18×18 system ($U=-4$) at disorder $W=1.3$: nearest-neighbor links D_{ij} (lines) colored from orange for strong correlations, to black for weaker correlations (close to cutoff $D_{ij}=0.45$), and disconnected for correlations below the threshold. Temperature changes from deep in the SC regime (a) to deep in the insulating regime (d). Local vortex density n_v (background) colored from dark green for low density, to bright yellow for high density, demonstrating the correlation between the local D_{ij} and the local n_v (see also fig. 4).

Results: percolation description. – Having established the relevance of the KT description for finite disorder, we now turn to check whether the same data can be described by the percolation picture. As with the granular system, one has to invoke a threshold to determine whether two sites in our lattice are coherently coupled. While our results are not sensitive to this particular choice, here we follow the standard procedure [20,28], where a link is disconnected when the Josephson coupling J is reduced below the physical temperature. Since for a single Josephson junction, $D_{ij}=I_1(J/T)/I_0(J/T)$, where $I_n(x)$ is a Bessel function of the first kind, then the threshold $J=T$ corresponds to $D_{ij}=0.45$. Thus, we set this value as a threshold for an existing coherence link between nearest neighbors, and then determine the temperature where edge-to-edge percolation is lost, T_p. Figure 3 demonstrates the connectivity of the network for temperatures from below to above the percolation temperature, where the existing links are colored by strength of D_{ij}, and the missing links are those with D_{ij} below the above threshold. The percolation temperature T_p can be determined for each disorder value, and, in fact, corresponds to an

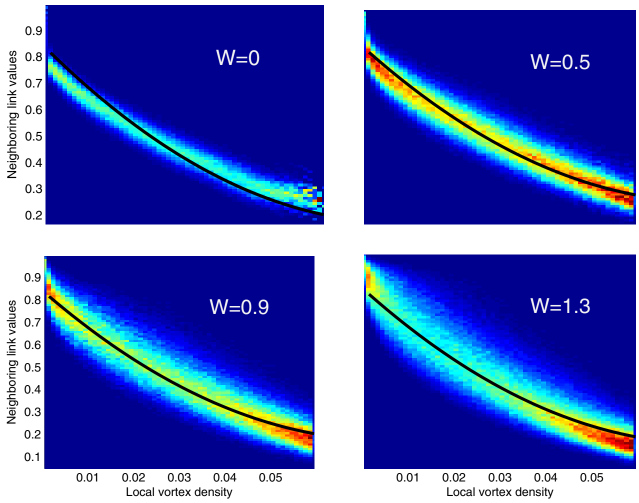


Fig. 4: The joint distribution of the local SC correlations and the local vortex density (normalized to unity at each vortex density). The strong correlation between the two values persists with increasing disorder, with the same functional form (solid line).

average link density of 1/2, consistent with bond percolation on a square lattice. T_p is also depicted as circles in fig. 1, demonstrating that it is indeed in the region where bulk correlations decay and vortices start to proliferate. In principle, of course, setting such a threshold will necessarily lead to a percolation transition. The fact that the vortex density at the percolation transition is independent of disorder is a strong indication of the applicability of our approach.

In order to quantify this last statement further, we have also plotted in fig. 3 the local vortex density n_v, in brighter shades of green for higher density. As can be clearly seen, as the local n_v increases, the neighboring D_{ij} decrease and disconnect. In fig. 4 we plot the dependence of the local D_{ij} on the local n_v, for different values of disorder. This dependence is observed to be independent of disorder (except for small corrections at zero disorder and a slightly wider distribution with increasing disorder), leading to the local D_{ij}, up to some small fluctuations, being a unique function of the local vortex density. This observation allows us to relate the two pictures: to destroy coherence locally, the local vortex density has to be high enough. Thus, in order for the percolation path of the D_{ij}'s to disconnect, a perpendicular line connecting points of n_v, larger than some threshold value, has to be formed. Consequently loss of percolation of the D_{ij} corresponds, in fact, to percolation of the vortices in the dual lattice in the perpendicular direction. Since this necessitates a particular density of vortices, it can only occur when vortices proliferate, *i.e.* at the KT transition. This point is further verified by marking the percolation temperature on the curves for the PAD exponent, fig. 2. For all values of disorder, this temperature corresponds to $\alpha \simeq 0.45$, just as the curves begin to smooth due to the finite size and exactly where the KT transition should occur.

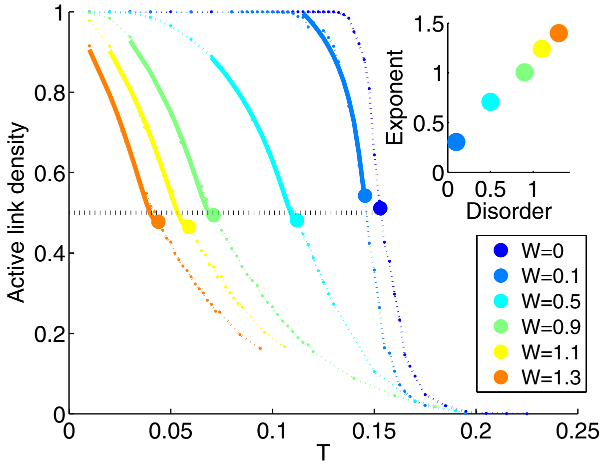


Fig. 5: Link density p as a function of temperature T. Large dots indicate T_p and agree well with $p = 0.5$ as expected from percolation theory. Solid lines are fits according to eq. (3). Inset: exponents ($\tilde{B}$ deduced from the fit).

Discussion and summary. – If these two transitions describe the same physics, then a curious question arises. For the KT transition the critical divergence of the SC correlation length ξ is expected to be $\xi(T) \sim e^{B/\sqrt{T_c/(T_c-T)}}$ where T_c the critical temperature and B is some non-universal number. On the other hand, near the percolation transition one expects $\xi(p) \sim (p_c - p)^{-\nu}$ where p is the link density (*i.e.* the concentration of links for which D_{ij} is above the threshold), p_c its critical value, and ν the correlation length critical exponent. Identifying the two transitions, *i.e.* the critical temperature T_c with the percolation temperature T_p, and the two critical behaviors, implies a very specific dependence of the link density on temperature,

$$p(T) = p_c + Ae^{-\tilde{B}\sqrt{(\frac{T_p}{T_p - T})}}. \qquad (3)$$

The dependence of p on T is displayed in fig. 5, along with the solid lines, given by eq. (3), with the resulting values of $\tilde{B}$ in the inset. The excellent agreement between the observed link density and the result of eq. (3) gives further credence to the intimate connection between the KT transition and the percolation transition. This peculiar dependence of the link density on temperature indicates that as the system approaches the KT transition, the local values of D_{ij} decrease rapidly, as the number of free vortices increases. Alternatively, when temperature is reduced through the critical temperature there is an avalanche of correlations through the system. Preliminary tests we have done on the disordered XY model, (in which the pair correlation amplitude is fixed and only the phases are allowed to fluctuate), show that such avalanching behavior cannot be fully captured in this model. A study of the significance of the amplitude fluctuations will be the subject of a future work.

The percolation description should be valid, as long as the variation of the local correlations from link to link is larger than the thermal fluctuations in the values of these correlations. This will ensure that the percolation path will be robust under such fluctuations. As the disorder decreases, the link-to-link variation decreases, and thus at some typical weak disorder, we expect the percolation picture to break down (the exact value of disorder where this happens depends on the exact numerical prefactors in our analysis). It should be pointed out that even for a perfectly clean system, we see variations of the local correlations from link to link, due to finite-size edge effects and our simulation errors. Interestingly, we find empirically that in the presence of such fluctuations, the percolation analysis remains valid all the way to zero disorder. Nevertheless, we have chosen to remove from fig. 5 the fit results for $W = 0$ to prevent possible confusion between the mechanisms generating such percolation behavior.

In this letter we have used the Metropolis Monte Carlo technique to make two separate claims. First, we present numerical evidence that the KT transition in the attractive Hubbard model persists into the high disorder regime, going beyond the range one can apply the Harris criterion. Second, we have shown that a percolation analysis is consistent with the KT results.

While the analysis presented here was for s-wave superconductors, it is interesting to note that experimental studies of the d-wave SC transition in thin YBCO films, gave evidence for both a percolative description [29] and a KT description [30] of the transition. Thus, we expect that our results can be generalized to other symmetries of the order parameter.

The KT transition is notoriously difficult to capture on finite lattices because of the exponential divergence of the correlation length, and we expect our results to suffer from finite-size effects. We have carried out tests on smaller lattices and values of the Hubbard U (U controls the SC coherence length) that indicate that as lattice size is increased (or coherence length decreased) the results flow towards the expected KT ones. Work is in progress towards increasing the lattice sizes and finite-size scaling analysis.

It would be interesting to investigate the critical behavior as one increases the thickness of the sample. Here one may expect a crossover from the KT behavior to the mean-field BCS description. Whether percolation still plays a role and how it is related to the BCS transition is a question that we plan to explore in the future.

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