Effects of strong disorder in strongly correlated superconductors

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We investigate the effect of strong disorder on a system with strong electronic repulsion. In the absence of disorder, the system has a *d*-wave superconducting ground state with strong non-BCS features due to its proximity to a Mott insulator. We find that while strong correlations make superconductivity in this system immune to weak disorder, superconductivity is destroyed efficiently when disorder strength is comparable to the effective bandwidth. The suppression of charge motion in regions of strong potential fluctuation leads to the formation of Mott insulating patches, which anchor a larger nonsuperconducting region around them. The system thus breaks into islands of Mott insulating and superconducting regions, with Anderson insulating regions occurring along the boundary of these regions. Thus, electronic correlation and disorder, when both are strong, aid each other in destroying superconductivity, in contrast to their competition at weak disorder. Our results shed light on why zinc impurities are efficient in destroying superconductivity in cuprates, even though it is robust to weaker impurities.

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Strong interparticle interactions and strong inhomogeneous potentials both tend to localize fermions. Strong repulsion can result in complete suppression of charge motion at commensurate filling, leading to a Mott insulator [1], while strong disorder causes decoherence of fermions, forming Anderson insulators [2]. There is evidence that weak disorder in the presence of strong interactions [3–7], as well as strong disorder in the presence of weak interactions [8], compete with each other, but the question of strong disorder in the presence of strong repulsion remains unresolved. The complex interplay of electronic interactions and disorder is crucial to understanding novel phenomena [9–15] beyond the standard paradigm of Fermi-liquid and BCS superconductivity.

A prototype of strongly interacting electronic systems is the cuprate high-T_c superconductors (HTSCs), which show *d*-wave superconductivity for a range of doping. Superconductivity in these systems is robust to disorder introduced by doping the parent compound. This is manifested in weak disorder dependence of T_c [16–18] and robust V-shaped low-energy density of states [19–21]. However, small concentrations of Zn impurities degrade T_c in these systems [22,23]. Zn provides a strong impurity potential, which is believed to be attractive [10,24], while dopant impurities are Born scatterers [25,26]. Thus a study of a strongly correlated superconductor in the presence of strong disorder potential is required to explain this discrepancy.

In this paper, we consider the effect of strong disorder on the strongly interacting *d*-wave superconducting (SC) state proximal to the Mott insulator. Our key findings are as follows: (i) While the presence of strong correlations makes superconductivity robust to weak disorder, at large disorder comparable to bandwidth, superconductivity is rapidly suppressed. (ii) At large disorder, Mott insulating patches anchor a surrounding region akin to Anderson insulator. With increasing disorder strength, these islands grow at the expense of local superconductivity. Thus at large disorder, strong correlation and strong potential fluctuations help each other in bringing about the sudden death of superconductivity. Our results thus explain both the robustness of a HTSC to dopant impurities and its sensitivity to Zn impurities within a single theory.

The study of disorder in the *d*-wave SC phase has a long history [27–29], with early treatment within inhomogeneous mean-field theory (IMT) [29,30], which ignores the effects of strong electronic repulsions. Strong Mott correlations and the consequent projection of the low-energy Hilbert space into states with no double occupancies [31–34] are, however, crucial to understanding the non-BCS character of the *d*-wave SC state in cuprates. A semianalytic approach, where the effects of projection are kept in terms of renormalization of Hamiltonian parameters, is the Gutzwiller approximation [35], which is known [36] to match the more sophisticated Monte Carlo results [33] for the homogeneous system. This approach is easily extended to a renormalized inhomogeneous mean-field theory (RIMT) [25,37–39], which captures the effects of both strong correlations and disorder in the system.

A surprising result of these attempts is that in spite of the *d*-wave nature of the order parameter, strong correlations make superconductivity robust up to moderate disorders [25,37–40]. This is ascribed to the electronic repulsions that modify the hopping amplitudes based on local density and smear out charge accumulation near deep potential wells, leading to a much weaker effective disorder [38]. The natural question arises: How does Anderson localization [2] occur in this system? Further, does the presence of strong repulsion, i.e., the largest energy scale in the problem, compete with or aid the localization of the electronic wave function for large disorder strengths?

In RIMT, strong interactions are treated nonperturbatively to obtain a low-energy effective Hamiltonian and disorder potential is added to this description afterwards, which fails to account for the fact that if the potential difference across a bond is much larger than the hopping scale, it is energetically unfavorable for the electron to hop across that bond. In this paper, we consider an extension of RIMT which builds in the absence of hopping across bonds with large potential difference across them, and thus includes the Anderson mechanism of localization in a more direct way. This approximation, called

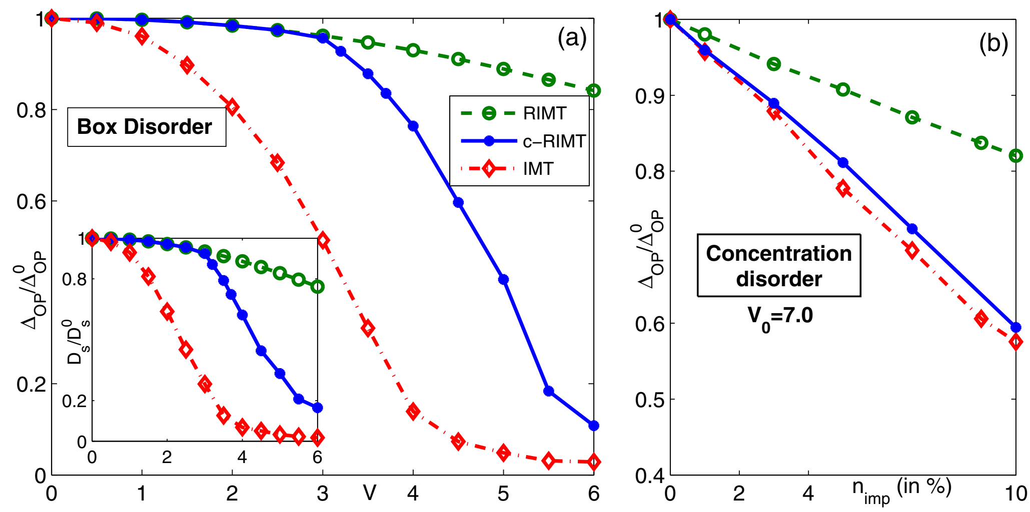

FIG. 1. (a) Δ_{OP} (normalized by its value at $V = 0$): Solid blue line represents c-RIMT results which cross over from its robust nature (for $V \leqslant 3$) to its crashing down for $3 \lesssim V \lesssim 6$. Δ_{OP} continues to be far less sensitive to V within RIMT (dashed green line), and shows a continuous fall starting right from small V within IMT scheme (dot-dashed red line). Thus, c-RIMT results interpolate between RIMT and IMT findings. Inset: Superfluid stiffness D_s shows a similar trend of Δ_{OP}, leading to its rapid destruction beyond V_c. (b) Evolution of Δ_{OP} with concentration of strong impurities in the c-RIMT method shows a better match with IMT than with RIMT results.

c-RIMT, allows us to smoothly interpolate between a robust SC at weak disorder to a patchy system of Mott and Anderson-like insulator at larger disorder strengths and shows the transition from immunity to sudden death of the SC.

Model and methods. We work with the disordered Hubbard model on a square lattice,

$$\mathcal{H} = -t\sum_{\langle ij\rangle\sigma}(c^\dagger_{i\sigma}c_{j\sigma} + \mathrm{H.c.}) + U\sum_i n_{i\uparrow}n_{i\downarrow}\sum_{i\sigma}(V_i - \mu)n_{i\sigma}. \tag{1}$$

Here, t and U are hopping and on-site repulsion energies, respectively, and $c^\dagger_{i\sigma}$ and $n_{i\sigma}$ are the creation and number operators for electrons on site i with spin σ. We work with $U = 12t$ and an average density, $\rho = 0.8$, so that the homogeneous system is a d-wave superconductor even in the presence of strong correlations. The nonmagnetic impurity potential V_i is taken from a uniform distribution between $-V/2$ and $V/2$. We emphasize that while we focus on $V \gtrsim t$, we always consider $V \ll U$, so that the projection constraints remain valid in our system [41].

At low energies, the homogeneous Hubbard model can be reduced to an effective $t - J$ model in the subspace where double occupancies are projected out through $\mathcal{P} = \prod_i(1 - n_{i\uparrow}n_{i\downarrow})$, by using a canonical transformation [42] about a local Hamiltonian. We carried out a similar procedure in the disordered model by including the disorder potential nonperturbatively in the local Hamiltonian. In this case, the potential difference across a bond provides an additional energy scale (other than U), which determines the effective Hamiltonian on that link. For weak potential difference across a link $\langle ij\rangle \in A$, $\Delta V_{ij} = |V_i - V_j| < V_c$, this gives the standard $t - J$ model with a superexchange scale $J_{ij} = (4t^2/U)(1 - \Delta V_{ij}^2/U^2)^{-1}$ [34,43–45] on that link. However, for $\Delta V_{ij} > V_c \sim t$, the electrons pay a large potential energy cost to hop across this bond and hence hopping on the corresponding link $\langle ij\rangle \in B$ is frozen, i.e., the bond is *cut off* from the system. The effective Hamiltonian is

$$\mathcal{H}_{\mathrm{eff}} = \sum_{\langle ij\rangle} J_{ij}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{n_i n_j}{4}\right) + \sum_i (V_i - \mu)n_i - t\sum_{\langle ij\rangle\in A\sigma}\mathcal{P}c^\dagger_{i\sigma}c_{j\sigma}\mathcal{P} + \sum_{\langle ij\rangle\in B\sigma}\frac{t^2}{V_i - V_j}(n_{j\sigma} - n_{i\sigma}). \tag{2}$$

The critical disorder $V_c \approx 2.8t$ is determined by balancing the kinetic energy gain with the potential energy loss for a single-impurity problem with a local potential V. We solve our modified "$t - J$" Hamiltonian within RIMT formalism, where $t_{ij} \to g^t_{ij}t_{ij}$ and $J_{ij} \to g^s_{ij}J_{ij}$ with $g^t_{ij} = 2[x_i x_j/(1 + x_i)(1 + x_j)]^{1/2}$ and $g^s_{ij} = 4/(1 + x_i)(1 + x_j)$. Here, x_i is the local hole doping which is determined self-consistently together with a Fock shift (τ_{ij}) and a d-wave pairing amplitude (Δ_{ij}) on each bond [see Supplemental Material (SM) [46] for details]. In this paper, we will present results on a 30×30 lattice (with a repeated zone scheme [38,47] used on 12×12 unit cells for better resolution and statistics; see SM [46]).

Demise of superconducting correlations. To look at the robustness of SC, we study the off-diagonal long-range order, $\Delta^2_{\mathrm{OP}} = \lim_{|i-j|\to\infty} F_{\delta,\delta'}(i - j)$, where $F_{\delta,\delta'}(i - j) = \langle B^\dagger_{i\delta}B_{j\delta'}\rangle$. Here, $B^\dagger_{i\delta} = (c^\dagger_{i\uparrow}c^\dagger_{i+\delta\downarrow} + c^\dagger_{i+\delta\uparrow}c^\dagger_{i\downarrow})$ is the singlet Cooper-pair creation operator on the bond $(i, i + \delta)$. An IMT calculation shows the demise of Δ_{OP}, as shown in Fig. 1(a) (dot-dashed line). Strong correlations in RIMT, where $\Delta_{\mathrm{OP}} \sim \sum_{\langle ij\rangle} g^t_{ij}\Delta_{ij}$, are known [25,38] to make superconductivity immune to disorder, as shown in Fig. 1(a) (dashed line). In this case, large local densities approaching unity lead to a decrease in the kinetic energy around those sites due to the renormalization factors. This nonlinear effect creates a repulsive potential and leads to a weak effective disorder in these systems, thereby making Δ_{OP} robust.

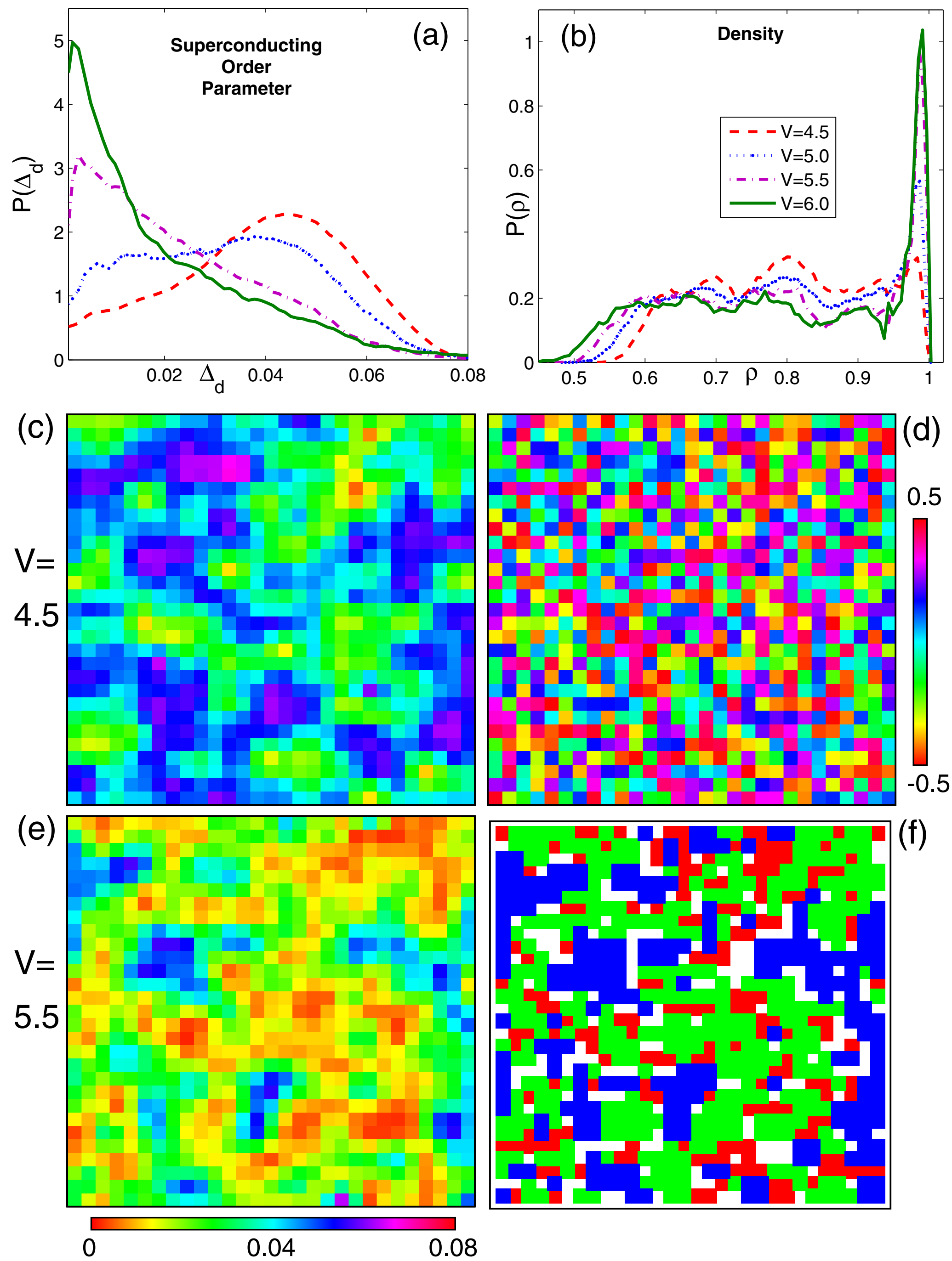

FIG. 2. Distribution of (a) Δ_d and (b) ρ for $V = 4.5$–6.0. $P(\Delta_d)$ broadens with increasing V with a peak at $\Delta_d = 0$, while Mott sites show up as a peak in $P(\rho \to 1)$ that sharpens with V. Color density plots of Δ_d on the lattice are shown for (c) $V = 4.5$ and (e) $V = 5.5$. Increasing V shrinks the blue regions forming superconducting "islands" in the matrix of nonsuperconducting regions. (d) Bare disorder profile. (f) The cross correlation of density and order parameter. In this map, (i) blue dots correspond to superconducting regions [$\Delta_d > 0.5\Delta_d(V = 0)$], (ii) red dots correspond to Mott regions ($\rho > 0.97$), and (iii) green dots correspond to non-SC, non-Mott region [$\Delta_d < 0.3\Delta_d(V = 0)$ and $\rho < 0.97$]. White patches in (f) are the regions that do not qualify the criteria to be any of the three primary regions.

Our c-RIMT calculation is identical to RIMT for $V \leqslant V_c$ as there are no cut bonds. However, in the range $V_c \leqslant V \leqslant 6.0$, up to 60% of kinetic links are frozen, and $\Delta_{\rm OP}$ depletes by nearly 90%. In this case, local potential wells, where the density is almost unity, are also accompanied by large potential differences in bonds connected to the wells, i.e., to frozen bonds. Thus the renormalization of the disorder potential around these wells is absent, leading to the formation of Mott insulating sites which anchor regions of large potential differences across bonds. In this region, hopping is severely suppressed due to large fluctuations in potential, causing a rapid destruction of coherence and superconductivity. Since this physics of losing transport is the same as in an Anderson insulator, we call these regions "Anderson insulating". We have

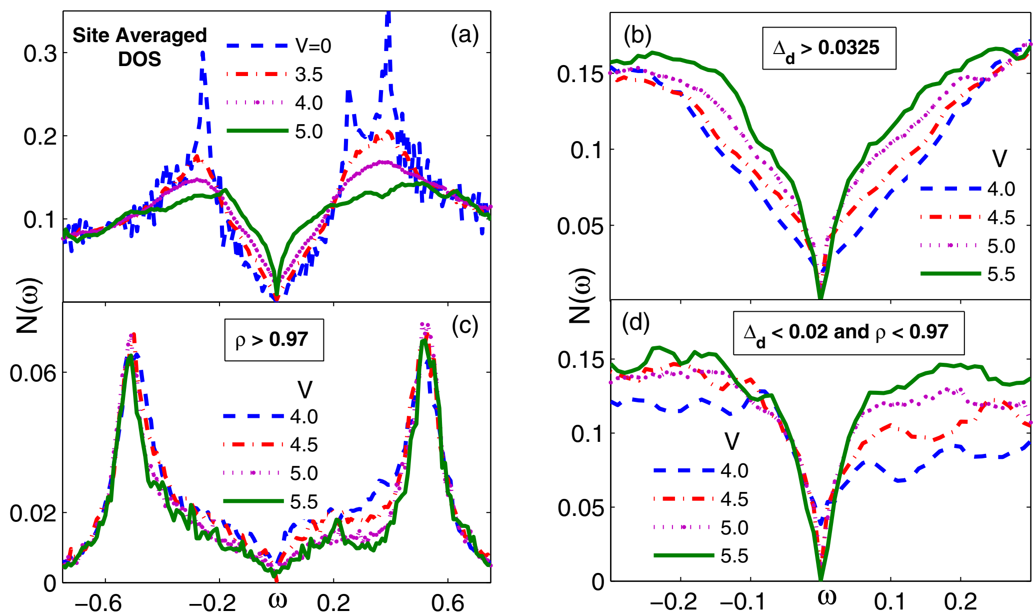

FIG. 3. (a) Site-averaged DOS, $N(\omega)$ showing filling up of midgap states for strong V and depletion of coherence peaks. (b)–(d) $N(\omega)$ in (b) superconducting regions, (c) Mott clusters, and (d) Anderson insulating region. The superconducting region shows a depleted coherence peak at $\omega = \pm 0.26$ for all V and Mott clusters show a spin gap at $\omega \sim J_{\rm eff}/2 \approx \pm 0.58$. The Anderson insulating region shows an otherwise flat DOS, except for a sharp gap feature at $|\omega| \leqslant 0.05$.

checked that a change in V_c merely gives a parallel shift to the trace $\Delta_{\rm OP}(V)$, without any qualitative modification.

The sudden demise of superconductivity for $V > V_c$ is also signaled by the decline of superfluid stiffness with V. The stiffness D_s [shown in the inset of Fig. 1(a)] is defined by

$$\frac{D_s}{\pi} = \langle -k_x \rangle - \Lambda_{xx}(q_x = 0, q_y \to 0, \omega = 0), \qquad (3)$$

where k_x is the kinetic energy along the x direction and Λ_{xx} is the long-wavelength limit of transverse (static) current-current correlation function [48].

We have also examined a model of randomly located impurities of strength V_0 on the $n_{\rm imp}$ fraction of sites, which is more relevant to Zn doping of cuprate HTSCs [24,49,50]. Zn impurities in HTSCs have traditionally been treated as strong repulsive potentials [51–53], although recent work has shown these impurities to be attractive [10,24]. We show here that for large repulsive $V_0 = 7.0$ ($> V_c$), the $n_{\rm imp}$ dependence of $\Delta_{\rm OP}$ follows the weak-coupling IMT behavior, rather than the strong-coupling RIMT trend, as shown in Fig. 1(b). In contrast, a healthy $\Delta_{\rm OP}$ persists up to a considerably large $n_{\rm imp}$ (similar to RIMT) for weaker $V_0 \lesssim 3$ [25,38,39]. In the SM [46], we show that for strongly attractive $V_0 = -4.0$, the behavior interpolates between the RIMT and IMT findings. Our results thus explain the loss of superconductivity in HTSCs with Zn impurities for both repulsive and attractive strengths.

Distribution of local order parameters. The picture we have painted above, i.e., at large V, disorder and interaction aid each other in killing SC, is validated when we look at the distribution of the local order parameter $\Delta_d(i) = \frac{1}{4}\sum_{j=n.n.}(-1)^{\delta_{j,i\pm\hat{y}}} g^t_{ij}\Delta_{ij}$ and the local density ρ_i as a function of V. This is plotted in Figs. 2(a) and 2(b) for several values of $V > V_c$. $P(\Delta_d)$ broadens with increasing V, developing a peak at $\Delta_d(i) \approx 0$, similar to IMT results [54,55] and in stark contrast to RIMT results [38], where the distribution forms narrow bands. However, unlike IMT, the importance of correlations becomes evident from Fig. 2(b) where the density distribution starts showing a strong peak at $\rho \approx 1$, indicating the importance of the formation of locally Mott insulating regions in the demise of superconductivity.

Our c-RIMT calculations afford us a granular view of the system in terms of spatial arrangements of different types of regions. To see this, the spatial distribution of $\Delta_d(i)$ is shown in Figs. 2(c) and 2(e) for $V = 4.5$ and $V = 5.5$, respectively. This shows the formation of superconducting and nonsuperconducting islands, with non-SC islands growing with disorder. However, a clearer picture emerges if we cross correlate the spatial distributions of order parameter and local densities and divide the sites into three representative classes: (i) Mott insulating sites, where local density $\rho(i) > 0.97$; (ii) superconducting sites, where $\Delta_d(i) > 0.033$; and (iii) sites with low order parameter ($\Delta_d(i) < 0.02$) and density not close to 1 [$\rho(i) < 0.97$], the non-SC, and non-Mott sites, which we will interpret as Anderson insulating patches. Figure 2(f) presents this cross-correlated data corresponding to the order parameter map in Fig. 2(e) for $V = 5.5$. Here the superconducting sites are colored blue, the Mott insulating sites are colored red, while the non-SC as well as non-Mott insulating sites are colored green. Figure 2(f) clearly shows that Mott insulating sites act as anchors around which the insulating patches nucleate. With increasing disorder, these Anderson insulating patches (green) form a network connecting the Mott sites. The fraction of both the red and green sites grow with disorder. Mott correlations and disorder potential aid each other in the limit of strong disorder to localize the electrons and kill superconductivity.

Local density of states. The three types of patches discussed above leave their signatures in the local density of states (DOS) at these points, $N(i,\omega) = g^t_{ii} \sum_n \{|u_{i,n}|^2\delta(\omega - E_n) + |v_{i,n}|^2\delta(\omega + E_n)\}$ [25,38], where $(u_{i,n}, v_{i,n})$ are the local Bogoliubov wave functions corresponding to energy eigenstates with energy E_n. In Fig. 3(a), we plot the DOS averaged over all sites in the system. At weak disorder, the V-shaped low-energy DOS is robust to disorder, which mainly affects the coherence peak at the gap edge. At larger disorder, superconducting coherence peaks deplete significantly and there is a filling of the d-wave gap, although a narrow gap exists even at strong disorder strength of $V = 5.0$.

The local density of states, averaged over the sites belonging to the three categories mentioned above, show distinct features of their own. In the superconducting regions [Fig. 3(b)], we find that the density of states continue to show the low-energy V-shaped feature characteristic of d-wave superconductors. As disorder is increased, the slope of the DOS with energy steepens at very low energy, indicating the transfer of spectral weight from high energies at the gap edge to the low energies. This is consistent with the fact that at strong disorder, the quasiparticles become heavier with V and hence disorder-averaged effective velocities v_F and v_Δ decrease. So the low-energy spectral weight $N(\omega) \sim \omega/v_F v_\Delta$ grows with V. In the Mott regions [Fig. 3(c)], there is a clear gap in the low-energy DOS with particle-hole symmetric sharp peaks at $\omega = \pm 0.58$, the location and line shape of which are robust to changes in V. This is because the Mott clusters are described by an effective Heisenberg Hamiltonian for localized spins in a basis without any double occupancy. The difference between the singlet and the triplet energies in this model is $\Delta_{\text{spin}} \sim J_{\text{eff}}$, the exchange coupling of that Hamiltonian, and is independent of the disorder. This is the scale that shows up in the DOS of the Mott regions, further confirming our association of these sites with Mott insulating patches. In the third region [Fig. 3(d)], we find a DOS which is flat at the energy scale of superconducting coherence peaks (similar to Anderson insulators, and hence the name), but features a tiny gap at very small $|\omega| \lesssim 0.05$. In these regions, the low-energy DOS first shows signs of gap filling at intermediate V, but as the disorder increases, there is a depletion of spectral weight at low energies, leading to a fully formed gap by $V = 5.0$. A thin gap in disordered d-wave SC had already been discussed in weak-coupling theories [29,30,52,56,57]. In addition, Coulomb repulsions are known to open up a gap in disordered systems [58–61]. Our results emphasize the role of strong correlations in the low-energy spectrum.

Conclusion. We have studied the effects of strong potential disorder on strongly interacting d-wave superconducting states in proximity to a Mott insulator. Using a c-RIMT method, which explicitly freezes hopping on bonds with large potential difference, we find that while strong correlations effectively compete against weak disorder to make superconductivity immune to disorder, at large disorder strengths, correlations and disorder aid each other, leading to the sudden demise of superconductivity. This is facilitated by the formation of Mott insulating patches, which anchor Anderson insulating patches around them.

We have not considered antiferromagnetic (AF) order [53] in the present calculation, which is present in the Mott insulating phase [62]. Short-range AF correlation, if generated, will be confined to the Mott patches and these patches already do not support SC. Hence this would not change the main conclusions about superconductivity in the system. Similar quantitative changes will occur with the inclusion of quantum phase fluctuations. However, the evolution of intertwined regions will survive and their distinct signatures in the DOS can be picked up by scanning tunneling microscopy.

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