# Enhancing superconductivity by disorder

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We study two mechanisms for enhancing the superconducting mean-field transition temperature $T_c$ by nonmagnetic disorder in both conventional (sign-preserving gaps) and unconventional (sign-changing gaps) superconductors (SCs). In the first scenario, relevant to multiband systems of both conventional and unconventional SCs, we demonstrate how favorable density-of-states enhancements driven by resonant states in off-Fermi-level bands lead to significant enhancements of $T_c$ in the condensate formed by the near-Fermi-level bands. The second scenario focuses on systems close to localization where random disorder-generated local density-of-states modulations cause a boosted $T_c$ even for conventional single-band SCs. We analyze the basic physics of both mechanisms within simplified models, and we discuss the relevance to existing materials.

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## I. INTRODUCTION

What happens to the superconducting transition temperature $T_c$ when the amount of disorder in a material is increased? This important question has been thoroughly studied both experimentally and theoretically, and the answer is known to depend on the nature of the disorder and the pairing symmetry of the superconductor (SC). The naive answer, in overall agreement with the bulk of previous studies, is that the $T_c$ drops, or at best remains unaffected. The latter possibility is the essence of Anderson's theorem stating that nonmagnetic disorder does not affect $T_c$ for conventional SCs [1]. This ceases to be true for unconventional SCs with sign-changing gap functions, and attention has been centered on measuring and explaining the $T_c$ suppression rate, i.e., $dT_c/dx$, where $x$ denotes the concentration of disorder [2].

There is, however, no fundamental principle preventing $T_c$ from rising with increased disorder, and experimental reports of disorder-enhanced $T_c$ exist in the literature [3–7]. It is also possible that part of the $T_c$ value in doped systems, such as cuprates and iron-pnictides, or inhomogeneous [8] or granular SCs [9] arise from the inhomogeneity itself. This idea is in line with a number of earlier theoretical studies concluding that in conventional SCs, disorder may under some circumstances enhance $T_c$ [10–17]. For example, in systems with short-range (screened) Coulomb interactions, $T_c$ may be strongly enhanced by Anderson localization, a property related to the multifractality of the wave functions in the disordered system [10,12,13]. Another series of studies have focused on periodically modulated SCs, and it was found that such systems may also exhibit larger $T_c$ than in the homogeneous case [18–23]. These results raise the following general question: under what circumstances does inhomogeneity boost $T_c$? Pinpointing such conditions may guide new disorder-engineered SCs with elevated $T_c$.

In this paper, we demonstrate that disorder-generated $T_c$ enhancements can happen for both conventional and unconventional SCs. Our study highlights the crucial role of spatial inhomogeneity and the generation of favorable local density-of-states (LDOS) enhancements generated by nonmagnetic disorder. This goes beyond the standard Abrikosov-Gor'kov (AG) treatment of disordered SCs, assuming a spatially uniform SC order parameter (OP) and constant DOS [24]. We study two separate scenarios for disorder-generated $T_c$ enhancements: (i) dilute disorder in multiband SCs, and (ii) dense disorder in conventional one-band SCs. In case (i), the multiband property is crucial; impurity resonant states generated by off-Fermi-level bands generate LDOS enhancements at the Fermi level $E_F$, which, through interband coupling, feeds into the near-Fermi-level bands important for SCs. As seen from Fig. 1(a), even for unconventional SCs this effect can overwhelm pair-breaking caused by nonmagnetic disorder, and it can raise $T_c$ well above that of the homogeneous system, $T_c^0$. In case (ii), the band structure is unimportant; LDOS modulations allow for regions with increased DOS in a densely disordered normal state, which can lead to enhanced $T_c$ [10,12,13]. Normally the insensitivity of the OP to disorder in conventional SCs is understood with reference to Anderson's theorem [1]. This, however, relies on dilute disorder and a spatially uniform OP and DOS. We do not include the harmful effect of longer-range Coulomb repulsion [25–28], restricting the relevance to sufficiently screened systems [12]. We also stress that our studies refer to the mean-field $T_c$, and that the role of phase fluctuations remains an important outstanding question.

To the best of our knowledge, scenario (i) has not been pointed out before, and for (ii) even though superconductivity near the localization threshold has been discussed before [11,29], only a limited set of previous studies have discussed the *favorable* effects of nonmagnetic disorder in conventional BCS superconductors [10,12,13,30,31]. In particular, Burmistrov *et al.* [12] studied the interplay of disorder and SCs within an Renormalization group analysis of the nonlinear $\sigma$-model, inferring that Anderson

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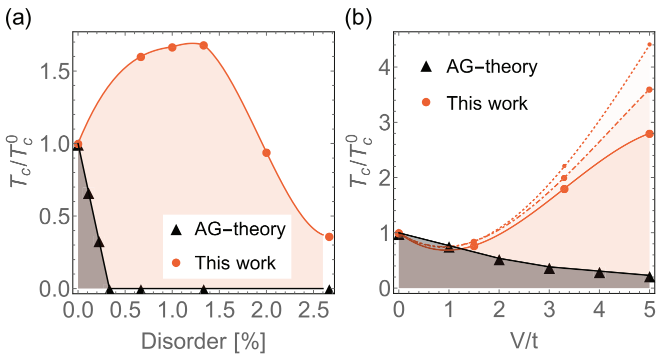


FIG. 1. Superconducting critical temperature $T_c/T_c^0$ in the presence of nonmagnetic disorder in (a) an unconventional multiband $s_\pm$ SC vs disorder concentration, and (b) a one-band $s$-wave SC with 15% disorder vs impurity strength $V$. The black curves show the results when disallowing spatial modulations of density and SC OP consistent with AG theory. The red curves show the self-consistent cases with spatial modulations of both quantities. In (b) $p = 2\%$ (dotted), $p = 5\%$ (line-dotted), and $p = 10\%$ (solid); see the text.

localization enhances $T_c$ for both two-dimensional (2D) and 3D systems. Notably this enhancement effect was not, however, observed in earlier numerical finite-size system simulations of the disordered attractive Hubbard model [32–34].

For unconventional SCs, the importance of allowing for spatial inhomogeneity in the SC OP has been pointed out for cuprates and heavy-fermion SCs [30,31,35–38]. In the case of cuprates, the observed $T_c$-suppression rate is considerably weaker than that dictated by AG theory [39–44], which was ascribed to the importance of a spatially adaptive SC condensate [30,35–37]. We note that the enhancement of SCs by disorder from the perspective of a local enhanced pairing interaction has also been discussed in the literature [45–51]. Within this scenario, the pairing interaction itself gets locally enhanced by disorder. Finally, we note that $T_c$ enhancements from disorder have also been discussed in the context of negative-$U$ centers [52–55].

## II. SCENARIO 1

For concreteness, we demonstrate the $T_c$-enhancement mechanism by a multiband model relevant to unconventional iron-based SCs (FeSCs),

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\mathrm{BCS}} + \mathcal{H}_{\mathrm{imp}}, \tag{1}$$

where $\mathcal{H}_0 = \sum_{\mu\nu\sigma ij}(t_{ij}^{\mu\nu} - \mu_0\delta_{ij}\delta_{\mu\nu})\hat{c}_{i\mu\sigma}^\dagger \hat{c}_{j\nu\sigma}$ denotes the hopping Hamiltonian with parameters adapted from the five-band model of Ref. [56]. The band structure consists of a Fermi surface with both electron and hole sheets with orbital $t_{2g}$ character, and lower-lying bands some of which exhibit predominantly $e_g$ character [56]. The operator $\hat{c}_{i\mu\sigma}^\dagger$ creates an electron at site $i$ in orbital state $\mu$ with spin $\sigma$, and $\mu_0$ is the chemical potential adjusting the average electron density $n$ of 6.0 electrons per site. We stress that the disorder does not provide additional carriers. The indices $\mu$ and $\nu$ denote the five iron orbitals ($d_{xz}$, $d_{yz}$, $d_{xy}$, $d_{x^2-y^2}$, $d_{3z^2-r^2}$). Superconductivity is included through the standard multiorbital singlet pairing BCS term, $\mathcal{H}_{\mathrm{BCS}} = \sum_{i\neq j,\mu\nu}[\Delta_{\mu\nu}\hat{c}_{i\mu\uparrow}^\dagger \hat{c}_{j\nu\downarrow}^\dagger +$ H.c.]. We fix the SC coupling constant $\Gamma = 0.2$ eV for attractive next-nearest-neighbor (NNN) intraorbital (and orbital-independent) pairing, producing a sign-changing $s\pm$ SC ground state with $\Delta_\mu^0 = (0.78, 0.78, 1.31, 0.063, 0.055)$ meV and $T_c^0 = 21$ K in the homogeneous case [62]. We will be interested in 3D materials such as cuprates and FeSCs, which are layered quasi-2D systems. Therefore, we can perform computationally simpler 2D calculations, with the understanding, however, that it is the interplanar coupling that supports a finite $T_c$. Finally, $\mathcal{H}_{\mathrm{imp}} = \sum_{\mu\sigma\{i\}} V\hat{c}_{i\mu\sigma}^\dagger \hat{c}_{i\mu\sigma}$ is the impurity term consisting of a set of impurity sites $\{i\}$ with on-site potential $V$ assumed, for simplicity, to be orbital-independent and of an intraorbital nature, in overall agreement with DFT findings [57,58]. We solve Eq. (1) by finding self-consistent solutions to its corresponding Bogoliubov–de Gennes (BdG) equations on $30 \times 30$ lattices with unrestricted density and OP fields with respect to all orbital and site degrees of freedom. For further computational details, we refer the reader to the supplemental material [59] and our earlier publications [60–62].

Applying conventional wisdom, any sign-changing OP should be quickly destroyed by disorder, and indeed an AG calculation with, e.g., $V = 0.725$ eV reveals that merely $\sim$0.5% disorder is sufficient to destroy the SC state, as shown in Fig. 1(a). This result can be obtained both by a standard T-matrix momentum-based approach [24,62–64] and by a real-space BdG calculation disallowing spatial modulations of density and SC. However, disorder *will* induce spatial modulations, and for systems such as FeSCs and cuprates, where the coherence length $\xi$ is a few nanometers, AG theory is no longer applicable. Consider for concreteness a 1.3% disorder concentration producing the nanoscale density modulations shown in Fig. 2(a). In Fig. 2(b) we plot the total normal state LDOS at $E_F$ $N(\mathbf{r})/N^0$, revealing large LDOS enhancements compared to the disorder-free system $N^0$. The formation of these enhancements near the disorder sites can be traced to the generation of resonant states in the off-Fermi-level $e_g$-dominated bands [60,65], which in turn drive a large enhancement of the SC OP in those orbitals, as seen in Fig. 2(c), which shows $\Delta_{e_g}/\Delta_{e_g}^0$ at $T/T_c^0 = 1.5$, i.e., well *above* the homogeneous $T_c^0$. Through the coupling to the $t_{2g}$ orbitals dominating the bands near $E_F$, this enhancement leaks into the OP $\Delta_{t_{2g}}$ of these orbitals, as seen in Fig. 2(d), thereby supporting the entire condensate to stay SC even at $T > T_c^0$. Therefore, allowing for full freedom in orbital and spatial indices, the resulting SC OP is remarkably robust. The final impurity configuration-averaged $T_c$ is shown by the red curve in Fig. 1(a). Here $T_c$ is defined as the highest $T$ where *all* sites acquire a finite OP. This definition of $T_c$ marks the onset of a fully connected SC, and it is also consistent with the onset of entropy loss and a concomitant step in the specific heat as seen from Figs. 2(e) and 2(f).

## III. TOY MODEL OF SCENARIO 1

To illuminate the mechanism for LDOS and $T_c$ enhancements presented above, we analyze a simplified two-band

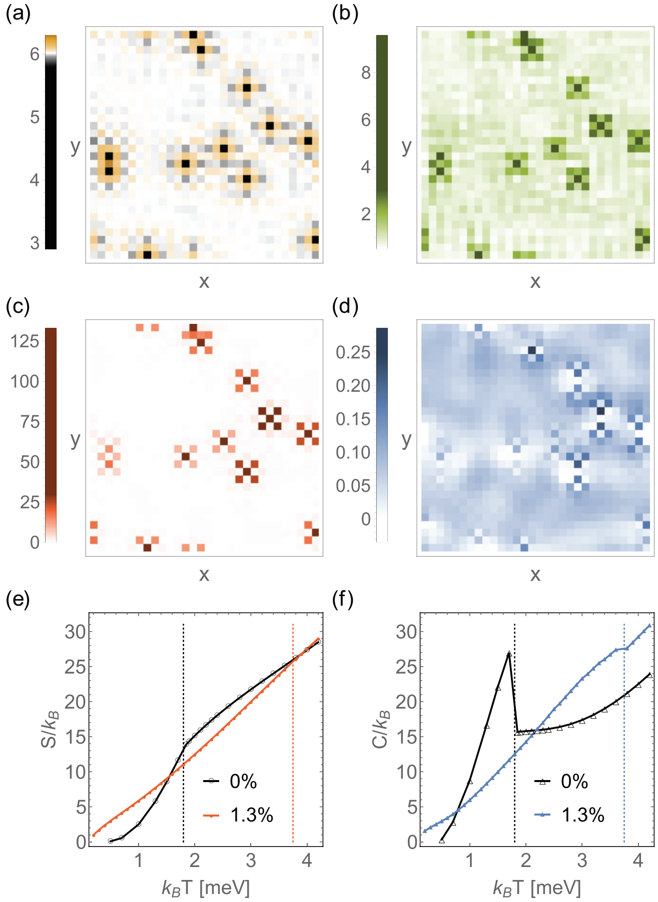


FIG. 2. (a) Real-space map of the total electron density in the presence of 1.3% disorder consisting of repulsive impurities, $V = 0.725$ eV. Total LDOS in the normal state $N(\mathbf{r}, \omega = 0)/N^0(\omega = 0)$ (b), self-consistent SC fields $\Delta_\mu(\mathbf{r})/\Delta^0_\mu$ at $T/T^0_c = 1.5$ for $d_{3z^2-r^2}$ (c) and $d_{xz}$ (d). The superscript 0 denotes parameters of the disorder-free system. $\Delta^0_\mu$ refers to the $T = 0$ gap value of orbital $\mu$ given by (0.78,0.78,1.31,0.063,0.055) meV in the basis of ($d_{xz}$, $d_{yz}$, $d_{xy}$, $d_{x^2-y^2}$, $d_{3z^2-r^2}$). (e,f) Entropy $S$ (e) and specific heat $C$ (f) vs $T$ comparing the disordered case (colored curves) with the homogeneous system (black curves).

lattice model,

$$\mathcal{H} = \sum_{\mu\nu\sigma\mathbf{k}} [\xi_\mu(\mathbf{k})\delta_{\mu\nu} + \gamma\delta_{\mu\bar{\nu}}]\hat{c}^\dagger_{\mathbf{k}\mu\sigma}\hat{c}_{\mathbf{k}\nu\sigma} + \sum_{\mu\mathbf{k}} \Delta_\mu \hat{c}^\dagger_{\mathbf{k}\mu\uparrow}\hat{c}^\dagger_{-\mathbf{k}\mu\downarrow} + \text{H.c.}, \tag{2}$$

with dispersion given by $\xi_\mu(\mathbf{k}) = -2t[\cos(k_x) + \cos(k_y)] - \epsilon_\mu$ with $\epsilon_a = t$ and $\epsilon_b = -6t$, and a coupling $\gamma$ between the two bands; see Fig. 3(a). Note that for simplicity for this toy model illustration we include a conventional on-site $s$-wave SC as opposed to the NNN pairing of the FeSCs case studied above. The connection to the previous section is that the $a$ ($b$) states dominate the near-Fermi-level (off-Fermi-level) bands corresponding to the $t_{2g}$ ($e_g$) dominated bands in the case of FeSCs.

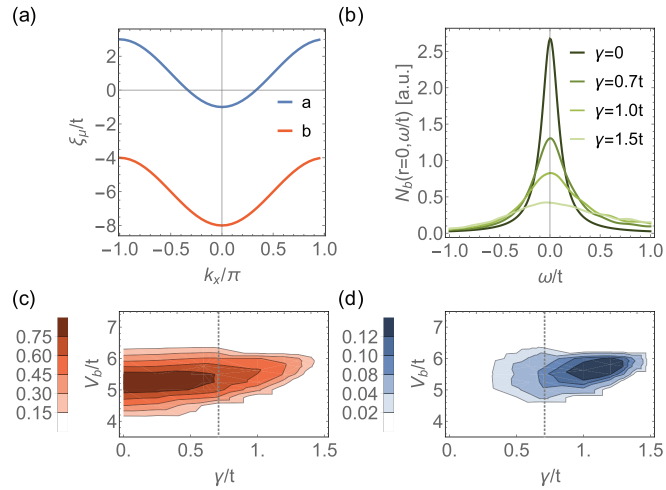


FIG. 3. (a) Band structure for the two-band toy model along $\mathbf{k} = (k_x, \pi/2)$. (b) $N_b(\mathbf{r}_0, \omega)$ for a resonant potential ($V_b = 1/\mathrm{Re}[g^0_b(\omega = 0)]$, $V_a = 0$) at the impurity site for different $\gamma$. Note that here we set $V_a = 0$ to most clearly demonstrate the origin of the $T_c$ enhancement. For the results in Fig. 2 we used a more realistic orbital-independent potential as stated above. The finite width at $\gamma = 0$ arises from an imposed broadening $\eta = T$. (c,d) Self-consistent induced fields $\Delta_\mu(\mathbf{r}_0) - \Delta^0_\mu$ in units of $t$ for bands $b$ (c) and $a$ (d) as a function of $V_b$ and $\gamma$ for on-site pairing $\Gamma = 1.93t$ and $k_B T = 0.1t$. The dotted lines in (c,d) show the $\gamma$ above which $\Delta^0_\mu = 0$ in the disorder-free system at this $T$.

In the presence of a pointlike impurity at the site $\mathbf{r}_0 = (0, 0)$, the full Green's function is given by

$$\hat{\mathcal{G}}(\mathbf{r}_i, \mathbf{r}_i; i\omega_n) = \hat{\mathcal{G}}^0(i\omega_n) + \hat{\mathcal{G}}^0(\mathbf{r}_i; i\omega_n)\hat{\mathcal{T}}(i\omega_n)\hat{\mathcal{G}}^0(-\mathbf{r}_i; i\omega_n), \tag{3}$$

where $\mathbf{r}_i$ denotes the position of the $i$th lattice site, and $\hat{\mathcal{T}}(i\omega_n) = (\mathbb{I} - \hat{V}\hat{\mathcal{G}}^0(i\omega_n))^{-1}\hat{V}$ and $\hat{\mathcal{G}}^0(i\omega_n) = \sum_{\mathbf{k}} \hat{\mathcal{G}}^0(\mathbf{k}; i\omega_n)$. To expose the $T_c$-enhancement mechanism, let us focus on $T > T^0_c$. In that case, and for a band-diagonal $\hat{V}$, the impurity states satisfy $\det[\mathbb{I} - \hat{V}\hat{G}^0(i\omega_n)] = \prod_\mu [1 - V_\mu g^0_\mu(i\omega_n)] = 0$, where $[g^0_\mu(i\omega_n)]^{-1} = i\omega_n - \xi_\mu - \gamma^2(i\omega_n - \xi_{\bar{\mu}})^{-1}$ refers to the local Green's function of band $\mu$ in the homogeneous normal state, and $\bar{\mu} \neq \mu$. Therefore, a band with $\mathrm{Im}[g^0_\mu(\Omega)] \approx 0$ exhibits a sharp resonant state at energy $\Omega$ for a potential satisfying $V_\mu = 1/\mathrm{Re}[g^0_\mu(\Omega)]$. Here, band $b$ is gapped around $E_F$ for small couplings $\gamma$ ($N^0_b \approx 0$), and it displays a correspondingly sharp resonant state at $E_F$ for $V_b = 1/\mathrm{Re}[g^0_b(\omega = 0)]$, as shown in Fig. 3(b). As $\gamma$ increases, the resonant state broadens due to the finite DOS of the $a$ band near $E_F$, and the LDOS enhancement $N_b$ drops.

The self-consistent gap at the impurity site obtained by solving the associated BdG equations on $40 \times 40$ lattices is shown in Figs. 3(c) and 3(d) for both bands $a$ and $b$ as a function of $\gamma$ and $V_b$. As seen from Fig. 3(c), the LDOS enhancement of $b$ induces a large corresponding local enhancement of $\Delta_b(\mathbf{r}_0) - \Delta^0_b$. However, there is no such LDOS increase for band $a$ (not shown), yet $\Delta_a(\mathbf{r}_0) - \Delta^0_a$ is also significantly enhanced as seen from Fig. 3(d). The origin of the increased $\Delta_a(\mathbf{r}_0)$ is found in the coupling to $\Delta_b(\mathbf{r}_0)$

as seen by linearizing the gap equation in the presence of the impurity at $\mathbf{r}_0$ for small $\gamma$, i.e., $\gamma, \Delta_a(\mathbf{r}_0) << \Delta_b(\mathbf{r}_0)$, obtaining

$$\Delta_a(\mathbf{r}_0) \propto V_b F(\Delta_b(\mathbf{r}_0))\gamma^2, \tag{4}$$

where $F(\Delta_b(\mathbf{r}_0))$ is an increasing function of $\Delta_b(\mathbf{r}_0)$ that vanishes linearly in the limit $\Delta_b(\mathbf{r}_0) \to 0$. Thus, the LDOS enhancement in $b$ directly increases $\Delta_b(\mathbf{r}_0)$, which indirectly boosts $\Delta_a(\mathbf{r}_0)$ through the coupling of the bands $\gamma \neq 0$ as seen by Eq. (4). We stress that this result illustrates the main mechanism behind the enhanced superconductivity seen in the FeSC case; see Fig. 2. Of course, in the realistic FeSC case used above there is a potential in all orbitals, which we excluded for simplicity in the toy model by setting $V_a = 0$. In the realistic FeSC case, what our calculations show is that the pair breaking in the $t_{2g}$ orbitals (produced by the potential in the $t_{2g}$ orbitals) is not strong enough to destroy the $T_c$ enhancement when the $e_g$ orbitals are "on resonance." At low $T$, $\Delta_{t_{2g}}$ is indeed suppressed near impurity sites, but the locally boosted $\Delta_{e_g}$ is still strong enough to uphold a finite $\Delta_{t_{2g}}$ at all sites in a range of $T$ above $T_c^0$, which is the important finding of our work.

From Figs. 3(c) and 3(d) it is evident that the $T_c$ enhancement hinges on the effect that resonant states are created near $E_F$, and that the coupling to the Fermi-level-relevant band is finite but weak enough not to destroy the resonant state itself. In materials with properties outside this "golden range," disorder operates as pair-breakers in unconventional SCs and lower $T_c$. There may be materials, however, where actual $T_c$ enhancements are not observed but very slow $T_c$-suppression rates are obtained due to the effect described above [62]. For FeSCs, such slow $T_c$-suppression rates have been measured for Ru-substituted LaOFeAs [66–68], and in fact the theoretical modelling of this material in Ref. [62] partly relied on the properties of the resonant states presented above. Finally, we note that interesting $T_c$ enhancements may also be expected in Kondo systems with $T_K > T_c$, since the screened moments produce large LDOS enhancements, in this case guaranteed at $E_F$. The anomalously high $T_c$ observed in the charge-Kondo system $Pb_{1-x}Tl_xTe$, where resonant impurity states were recently shown to be crucial for the SC phase, may be related to the scenario presented here [69–71].

## IV. SCENARIO 2

The above results raise the question of what happens to $T_c$ in conventional SCs with a sign-preserving OP. For the cases shown in Figs. 1(a) and 2, the answer is that the $T_c$ enhancement is even more pronounced because of the absence of pair-breaking. However, even for disorder strengths off-resonance, a substantial $T_c$ enhancement exists for sign-preserving gap functions with large enough disorder concentrations $n_{\mathrm{imp}}$ [10,12,13]. This can be demonstrated by the one-band attractive Hubbard model with NN (NNN) hopping $t$ ($t' = -0.3t$), filling 0.85, and $s$-wave OP stabilized by on-site attraction $|U| = 0.8t$, producing a $\Delta^0 = 0.022t$ at $T = 0$, and $k_B T_c^0 = 0.0135t$. In Figs. 4(a)–4(l) we show the $T$ dependence of $\Delta(\mathbf{r})/\Delta^0$ in real-space $40 \times 40$ maps for a 15% disordered system with different impurity strengths $V$. As seen, for strong enough $V$ the disorder stabilizes large regions of finite $\Delta(\mathbf{r})$

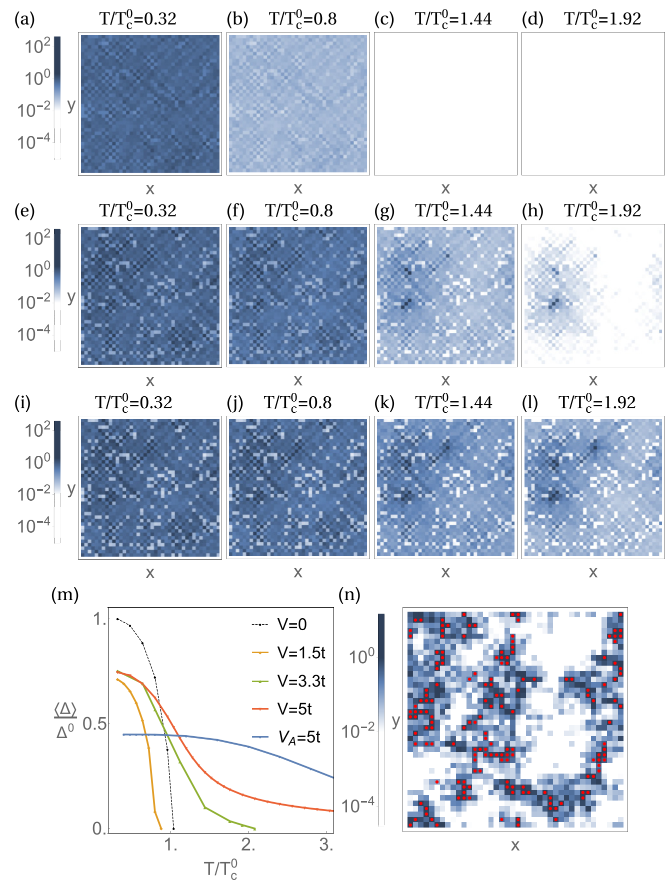


FIG. 4. (a)–(l) Real-space maps of $\Delta(\mathbf{r})/\Delta^0$ vs $T$ for a 15% disordered system with varying impurity strength $V = 1.5t$ (a)–(d), $V = 3.3t$ (e)–(h), $V = 5t$ (i)–(l) for a conventional $s$-wave SC in a one-band model. (m) Spatially averaged SC OP $\langle\Delta\rangle/\Delta^0$ vs $T$ for varying disorder strength $V$, and for Anderson disorder with $V_A \in [-5, 5]t$ (blue curve). The clean case is shown by the black curve. (n) Real-space map of $\Delta(\mathbf{r})/\Delta^0$ at $T/T_c^0 = 1.93$ for the case of Anderson disorder. The red dots indicate sites with large $T_c(\mathbf{r})/T_c^0 \propto \exp\{-1/[|U|N(\mathbf{r})]\}/\exp[-1/(|U|N^0)] > 0.4$, displaying the clear correlation between the local LDOS enhancements and the increased SC.

well above $T_c^0$. In Fig. 4(m) we show the spatially averaged $\Delta(\mathbf{r})$ as a function of $T$, clearly demonstrating the enhanced SC for the disordered case. We have also studied Anderson disorder and found similar behavior, shown by the blue curve in Fig. 4(m). The origin of the $T_c$ enhancement is favorable centers of enhanced LDOS as seen from Fig. 4(n), showing the strong correlation between $\Delta(\mathbf{r})$ and $N(\mathbf{r})$.

Unlike scenario 1, for the results in Fig. 4 the high level of disorder prevents one from defining $T_c$ in terms of simple steps or discontinuities in thermodynamic quantities. The spatially averaged $\langle\Delta\rangle$ also does not easily allow for a sound definition of $T_c$ because the OP breaks up into disconnected regions at large $T$. Therefore, for this case we define $T_c$ as the highest $T$ where all edges of the system are fully connected by gap amplitudes of at least $p$% of $\Delta^0$, the $T = 0$ homogeneous OP. Figure 1(b) shows the resulting $T_c/T_c^0$ curves for different $p$ thresholds, with a substantial upturn for strong disorder. Obviously the value of $p$ affects the magnitude of the $T_c$

enhancement, but not the existence of a disorder-generated $T_c$ enhancement itself.

For the cases shown in Fig. 4, one may estimate the mean free path $l = v_F\tau$ from the scattering rate $\tau^{-1} = 2\pi n_{\rm imp} N^0 V^2/(1+[N^0V]^2)$, yielding that for the cases with $V \gtrsim (2-3)t$, $l \sim$ 1–2 lattice spacings. Therefore, these cases approach the Anderson localized limit, and the existence of a $T_c$ enhancement is consistent with the findings by Burmistrov *et al.* [12]. We ascribe the reason that $T_c$ enhancements were not previously seen in numerical simulations to the small system size and very large SC OP used in those studies [32–34].

It remains interesting to extend the current studies to include phase fluctuations, potentially important for inhomogeneous systems with regions of low superfluid density [72]. In general, phase fluctuations lower the mean-field $T_c$, but the reduction depends strongly on dimensionality and the spatial structure of the modulations driving the inhomogeneity. For 3D systems, and when $\xi$ is of the same scale as the disorder-generated density modulations, the mean-field $T_c$ is not expected to be strongly affected by phase fluctuations [12,18,72].

We have studied mean-field $T_c$ enhancements in both conventional and unconventional superconductors from disordering with nonmagnetic impurities. Our results suggest a path to engineer systems with larger $T_c$ by introducing suitable amounts of disorder. We focused on superconductivity, but similar effects may also be expected for systems with other preferred symmetry breaking.

## ACKNOWLEDGMENTS

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