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Raising the critical temperature by disorder in unconventional superconductors mediated by spin fluctuations

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We propose a mechanism whereby disorder can enhance the transition temperature $T_c$ of an unconventional superconductor with pairing driven by exchange of spin fluctuations. The theory is based on a self-consistent real space treatment of pairing in the disordered one-band Hubbard model. It has been demonstrated before that impurities can enhance pairing by softening the spin fluctuations locally; here, we consider the competing effect of pair-breaking by the screened Coulomb potential also present. We show that depending on the impurity potential strength and proximity to magnetic order, this mechanism results in a weakening of the disorder-dependent $T_c$-suppression rate expected from Abrikosov-Gor’kov theory, or even in disorder-generated $T_c$ enhancements.

Introduction. Disorder has been used as a powerful probe of superconducting order since a theoretical framework for interpreting its effects was provided by Anderson[1] and Abrikosov-Gor’kov[2] (AG). Within translation-invariant effective medium theories of this type, disorder generally suppresses the critical temperature $T_c$, with the exception of nonmagnetic impurities in an isotropic, $s$-wave paired superconductor, where $T_c$ is impervious to disorder until the mean free path becomes of order an atomic spacing and localization effects set in. The theory applies equally well to unconventional superconductors, where even nonmagnetic impurities are typically pair-breaking. While it does not describe $T_c$ suppression quantitatively in strongly coupled systems like cuprates, where Zn causes an initial suppression 2-3 times slower than the AG-rate[3–7], still almost universally $T_c$ decreases upon addition of disorder.

There are, however, a few special situations where this conclusion does not apply[8–25]. We do not consider trivial $T_c$ enhancements, e.g. impurities that dope the system and thus change the Fermi surface, but rather physical effects of disorder itself not included in the AG approach for a simple BCS superconductor. For example, $T_c$ can be enhanced by disorder if the superconductor is competing with another type of order, e.g. a density wave, which is more sensitive to disorder than the superconductor [9–12]. Several authors have argued recently that $T_c$ can be increased by disorder at levels where localization becomes important due to the multifractality of electronic wave functions[13–15]. Related studies of $T_c$ enhancements exist also in the fields of granular and phase separated systems[16–18]. Finally we note a study where modulating the local density of states by disorder in several possible scenarios can yield an enhancement of $T_c$[19].

Another class of studies have focused on effects of inhomogeneity in the pairing interaction itself without reference to any particular microscopic mechanism to create it[20–25]. From these studies, it is known that systems with a modulated pair interaction have a $T_c$ that may be enhanced relative to a system with a homogeneous pairing interaction fixed to the average in the modulated system[20–24]. Most theories of this type that rely on pairing inhomogeneity are somewhat idealized, however, since if the fluctuating pair interactions indeed arise from disorder, impurities or defects will inevitably create a concomitant screened Coulomb potential component that will tend to break pairs, particularly in unconventional superconductors.

In this work, we propose a different mechanism for disorder-generated $T_c$-enhancements in unconventional superconductors. We study the effect of atomic scale defects on local spin fluctuations giving rise to $d$-wave pairing, but include pair-breaking effects through self-consistent studies of finite concentrations of disorder. From previous studies, it is known that a single nonmagnetic impurity softens spin fluctuations locally[26–28], which favors $d$-wave pairing within a spin-fluctuation mediated scenario[29, 30]. Note that the transfer of spectral weight is from typical normal state fluctuation energies of order $\sim t$ down to a fraction thereof; we do not treat dynamical pair-breaking effects known to occur when the fluctuations occur on the scale of $T_c$ itself[31]. In terms of thermodynamics, however, such disorder-enhanced local pairing must compete with the inevitable pair-breaking effect of the impurities, and it is unclear which effect dominates $T_c$ for finite disorder concentrations $p_{imp}$. As shown in Fig. 1, we find that the locally enhanced pairing scenario generally predicts significantly slower $T_c$-suppression rates, and can even in some circumstances support a remarkable disorder-generated $T_c$-enhancement. As seen from Fig. 1, this unusual behavior of $T_c$ is very different from that predicted by AG theory, which yields for a $d$-wave superconductor a rapid, monotonically decreasing $T_c$ with increasing disorder.

Specific to the one-band Hubbard model, we note the results of a recent dynamical cluster study of $d$-wave correlations finding a small initial enhancement of $T_c$ with
$p_{\text{imp}}$, and attributed it to an increase of the local exchange $J$ in a strong-coupling picture[32]. This study left unclear, however, under what circumstances a system described by such a theory would exhibit conventional AG-like $T_c$ suppression with increasing $p_{\text{imp}}$, and when it will deviate strongly. Under what circumstances can $T_c$ really be enhanced by the addition of disorder? The present study was motivated in part by this theoretical question, and by recent electron irradiation experiments performed on FeSe[33], which reported a 10% rise in $T_c$ under circumstances that precluded an explanation in terms of doping or chemical pressure. Local pinning of spin fluctuations by irradiation-induced defects was one of the possible mechanisms discussed, but without reference to the possible pair-breaking effects that such defects could induce.

Model and Method. The starting point is the one-band Hubbard model

$$H = -\sum_{i,j,\sigma} t_{i,j} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} U n_{i\sigma} n_{i\bar{\sigma}} - \sum_{i\sigma} \mu n_{i\sigma}$$

$$+ \sum_{i,\text{imp},\sigma} V_{\text{imp}} \delta_{i\text{imp},\sigma} n_{i\sigma},$$

with a concentration $p_{\text{imp}}$ of nonmagnetic impurities of strength $V_{\text{imp}}$ at random sites placed at positions $i_{\text{imp}}$.

The operator $c_{i\sigma}^\dagger$ refers to creation of an electron with spin $\sigma$ at lattice site $i$, and $n_{i\sigma}$ is the number operator of spin $\sigma$ particles at site $i$. The hopping elements $t_{i,j}$ include nearest neighbor (NN) $t = 1$, and next-nearest neighbor (NNN) $t' = -0.3$, and the system is hole-doped by $x = 0.15$, generating a standard Fermi surface relevant to cuprates. In the homogeneous case, an on-site repulsive Coulomb interaction $U$ gives rise to an effective attraction for superconductivity in the $d$-wave singlet channel as shown by weak-coupling spin-fluctuation theories [34, 35], and in qualitative agreement with strong-coupling numerical studies[36]. In the dirty case, however, $U$ modifies the charge and spin densities as well as the effective electron-electron interaction locally. To capture these effects, we first treat the Hubbard Hamiltonian at the mean-field level

$$H_0 = -\sum_{i,j,\sigma} t_{i,j} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} (U n_{i\sigma} - \mu) n_{i\bar{\sigma}}$$

$$+ \sum_{i,\text{imp},\sigma} V_{\text{imp}} \delta_{i,\text{imp}} n_{i\sigma},$$

in order to determine the electronic densities self-consistently in the presence of the disorder. Given the self-consistent densities, the associated spatially modulated effective superconducting pairing arising from higher order interactions in $U$ is determined by [29]

$$V_{ij}^{\text{eff}} = U + \frac{U^3 \chi^2_0}{1 - U^2 \chi^2_0} \sum_{i,j} f(E_{m\sigma}) - f(E_{m\bar{\sigma}}) \frac{E_{m\sigma} - E_{m\bar{\sigma}} + i\eta}{E_{m\sigma} - E_{m\bar{\sigma}} + i\eta}.$$  (3)

The susceptibility in (3) is a real space matrix given by

$$\chi_{ij}^{\sigma\bar{\sigma}} = \sum_{m,n} u_{m\sigma} u_{m\bar{\sigma}} u_{n\sigma} u_{n\bar{\sigma}} f(E_{m\sigma}) - f(E_{m\bar{\sigma}}) \frac{E_{m\sigma} - E_{m\bar{\sigma}} + i\eta}{E_{m\sigma} - E_{m\bar{\sigma}} + i\eta},$$  (4)

in terms of the eigenvectors $u_{m\sigma}$ and eigenvalues $E_{m\sigma}$ of Eq.(2). Thus, $u_{n\sigma}$ denotes the value of the eigenfunction $u_{m\sigma}$ on site $i$. Note that, as is customary, the pairing interaction is assumed to be fully determined by the properties of the paramagnetic normal state.

After obtaining the effective self-consistent spin-fluctuation mediated pairing kernel in real space, the densities $\langle n_{i\sigma}\rangle$ and superconducting gap values $\Delta_{ij}$ are calculated via a second self-consistency loop from the full mean-field Hamiltonian given by

$$H_{\text{SC}} = H_0 + \sum_{i,j} \left[ \Delta_{ij} c_{i\sigma}^\dagger c_{j\bar{\sigma}} + \text{H.c.} \right]$$  (5)

In the calculation of the singlet gaps

$$\Delta_{ij} = -\frac{V_{ij}^{\text{eff}}}{2} \sum_n \left[ u_{n\sigma} u_{n\bar{\sigma}} + u_{n\bar{\sigma}} u_{n\sigma} \right] \tanh(E_n / 2k_B T),$$

we account for superconducting links $\Delta_{i,i+\delta}$, where $\pm \delta \in \{0, \hat{x}, \hat{y}, 2\hat{x}, 2\hat{y}, \hat{x} + \hat{y}, \hat{x} - \hat{y}\}$. We refer to the above procedure as the "local pairing scenario". We find that in general, the NN links supporting $d$-wave superconductivity dominates, but higher order $d$-wave and subsidiary on-site order is induced in the vicinity of the impurities. We stress that the model contains only the free parameters $U$ and $V_{\text{imp}}$. For the results below we fix $U = 1.9$, and explore the dependence of $T_c$ on $V_{\text{imp}}$ and $p_{\text{imp}}$. 

FIG. 1. Critical superconducting transition temperature $T_c$ as a function of disorder concentration for nonmagnetic impurities of strength $V_{\text{imp}} = 2$ in $d$-wave superconductors of Coulomb interaction strength $U = 1.9$ (blue curve) and $U = 1.83$ (magenta curve). Results are averaged over four different impurity configurations. The black line shows the Abrikosov-Gorkov result corresponding to the $U = 1.9$ case.
The results from the local pairing scenario are compared to standard AG theory of nonmagnetic impurities in unconventional (sign-changing) superconductors, where \( T_c \) is obtained from the well known expression

\[
\ln \left( \frac{T_c}{T_{c,0}} \right) = \Psi \left( \frac{1}{2} \right) - \Psi \left( \frac{1}{2} + \frac{1}{4\pi T_c \tau} \right). \tag{6}
\]

The normal state scattering rate in the \( T \)-matrix approximation is given by \([37, 38]\)

\[
\frac{1}{\tau} = 2\pi p_{\text{imp}} \frac{V_{\text{imp}}^2 N(0)}{1 + (V_{\text{imp}} N(0))^2}, \tag{7}
\]

where \( N(0) \) is the density of states at the Fermi level and \( \Psi(x) \) refers to the digamma function.

**Results.** For inhomogeneous systems, there are various definitions of \( T_c \) that one might adopt. For example, one could define \( T_c \) by the temperature at which the first island becomes superconducting upon cooling. Instead, we adopt a more experimentally relevant definition: \( T_c \) is the highest temperature where more than 60% of the lattice sites possess a gap value that exceeds 20% of \( \Delta(0) \), where \( \Delta(0) \) is the gap of the clean system at \( T = 0 \) and 0.20\( \Delta(0) \) is of the order of the level spacing in our simulation, i.e. the bandwidth divided by system size \( N^2 \) with \( N = 30 \). This rather conservative definition captures the situation where all superconducting sites of the 2D lattice are connected in the present case of randomly placed point-like disorder. Note our calculations are strictly at the level of inhomogeneous (BCS) mean field theory, and effects of fluctuations are therefore not included. These fluctuations may be expected to suppress the mean field \( T_c \) significantly in situations where the length scale of the inhomogeneity is larger than the coherence length[20].

Local gap maps at temperatures both below and above \( T_c \) are shown in Fig. 2(a-d) for a system with 8% impurities of strength \( V_{\text{imp}} = 2 \). We show the magnitude of the superconducting \( d \)-wave links calculated as \( |\Delta_i| = \frac{1}{2} (\Delta_i(\hat{x}) - \Delta_i(\hat{y}) + \Delta_i(-\hat{x}) + \Delta_i(-\hat{y})) \), where \( \hat{x} \) (\( \hat{y} \)) denotes the unit vector along the \( x \)-axis (\( y \)-axis). At low \( T_c \), large gap enhancements in the vicinity of the impurity sites are clearly visible as seen from Fig. 2(a). Upon increasing temperature the order is diminished and destroyed at sites farthest away from the impurities until eventually the superconducting regions become fully separated in space above \( T_c \) as seen in Fig. 2(d).

Due to the inhomogeneity of the superconducting phase, the thermodynamic response of the phase transition is smeared. We calculate the specific heat from the derivative of the entropy \( C = T \partial S/\partial T \), where

\[
S = -2k_B \sum_{E_n > 0} f(E_n) \ln(f(E_n)) + f(-E_n) \ln(f(-E_n)).
\]

The superconducting transition of the clean system is clearly manifested by a jump in the specific heat at \( T_c \) as shown in Fig. 2(e) by the black line. By contrast, in the dirty system with 8% disorder, a broad peak marks the transition at a temperature that agrees well with the definition of \( T_c \) stated above [39].

In Fig. 1 we show the full evolution of \( T_c \) versus \( p_{\text{imp}} \) for the case with \( V_{\text{imp}} = 2 \). The \( T_c \)-enhancement is clearly visible in an extended range of disorder concentrations in the case with \( U = 1.9 \). For weaker \( U \), \( T_c \) is suppressed for all \( p_{\text{imp}} \) but still exhibits a large critical impurity concentration. In fact, within the local pairing scenario the superconductor is much more robust to impurities than predicted by AG theory, easily supporting a superconducting state to an order of magnitude more disorder as seen from Fig. 1. Figure 1 thus demonstrates that indeed the local pairing enhancements caused by the softened spin fluctuations can overcome the inevitable pair-breaking for a significant range of \( p_{\text{imp}} \). A similar study for attractive impurities [40] reveals that the \( T_c \)-suppression rate remains weaker than prescribed by AG-theory, but no disorder-generated \( T_c \)-enhancement exists in the case of \( V_{\text{imp}} < 0 \) for the cuprate-like band structure studied here.

In order to understand the origin of the \( T_c \) enhancement of Fig. 1, we show in Fig. 3(a) the increase in NN attraction \( \frac{1}{4} \left[ V_{\text{eff}}^{i,i+i_x} + V_{\text{eff}}^{i,i+i_y} + V_{\text{eff}}^{i,i-i_x} + V_{\text{eff}}^{i,i-i_y} \right] \) for a system of 8% impurities, still with \( V_{\text{imp}} = 2 \). We calculate
the pairing of the dirty system $V_{\text{eff}}(T)$ at $T = 1.2T_{c,0}$, where $T_{c,0}$ is the critical temperature of the clean system and subtract the NN attraction of the pure system $V_{0,\text{eff}}(T_{c,0})$. We stress that the attraction in the dark regions of Fig. 3(a) is not in itself sufficient to support superconductivity (since $T > T_{c,0}$). Nevertheless, the system displays a non-zero d-wave gap in these regions, as seen from Fig. 3(b), due to proximity coupling to the regions of enhanced pairing, which thereby boost the superconducting condensate of the entire system. Such local regions favorable to pairing can be understood from certain advantageous clustering of impurities, illustrated in Fig. 3(c) and (d). For example, a constructive interference of two impurities forming diagonal dimers lead to gap enhancements of $\sim 200\%$ with 6 sites involved, as compared to the $\sim 50\%$ enhancement effect of four sites around a single impurity. Diagonal structures of more than two impurities are even more advantageous and systems with such structures lead to an even larger increase in local pairing.

In Fig. 4(a) we show the results of the $T_c$-suppression rate for the case with a weaker impurity potential $V_{\text{imp}} = 1$. As expected, weaker scatterers raise the critical disorder concentration. However, it is found that 1) there remains a substantial difference between the AG result and the local pairing scenario, and 2) the $T_c$ enhancement is nearly eliminated. There are two reasons for property 1): correlation-induced screening [32, 41–46], and local pairing enhancements. By performing the real-space calculation for the case $U = 0$, while including a constant nearest-neighbor attraction, one almost quantitatively obtains the AG result, despite the local suppressions of the gap. However, as an instructive intermediate step we have calculated the $T_c$-suppression when $U \neq 0$, but without local pairing modulations, as shown by the red curve in Fig. 4(a). A comparison of gap maps in Fig. 4(b) and in Fig. 4(c) reveals a less modulated gap for the case $U \neq 0$ than for $U = 0$. This correlation-induced screening arises from the induced density modulations at the impurity site as seen by rewriting the density mean-field term as

$$\sum_{i\sigma} U \langle n_{i\sigma} \rangle n_{i\bar{\sigma}} = \sum_{i\sigma} U [\Delta n_{i\sigma} n_{i\bar{\sigma}} + \frac{U}{2} (n_{i\sigma} + n_{i\bar{\sigma}})],$$

where $\Delta n_{i} = \langle n_{i} \rangle - n_{0}$, and $n_{0}$ denotes the density of the clean system. The presence of a local repulsive potential repels electrons from the impurity site creating a $\Delta n_{\text{imp}} = \langle n_{\text{imp}} \rangle - n_{0} < 0$. This reduces the effective impurity potential $[V_{\text{imp}} + U \Delta n_{\text{imp}}]$, an effect most relevant to weak impurity potentials, and reduces their $T_c$-suppression rate. The opposite effect happens for magnetic impurities, which are anti-screened by $U[47]$. The $T_c$-suppression rate is further decreased when the electronic correlations are included also in the effective pairing interaction in the inhomogeneous system, as seen from Fig. 4(a), and the comparative gap map in Fig. 4(d). We note that the value of $U$ at the impurity sites affects the screening effect, but does not modify $T_c$ in the local
pairing approach since the pairing enhancement is not occurring at the impurity sites, but in their vicinity.

Regarding point 2) above, stronger individual impurities of $V_{\text{imp}} \simeq 2$ lead to larger local pairing on neighboring sites compared to $V_{\text{imp}} \leq 1$. At small to moderate concentrations $p_{\text{imp}}$, stronger impurities are therefore more beneficial for the global $T_c$. However, a larger impurity potential is more pair-breaking, and therefore at large $p_{\text{imp}}$, the pair-breaking effect becomes dominant in agreement with the decreasing critical impurity concentration for larger impurity potentials. In the unitary limit the density is fully suppressed at the impurity sites, and $T_c$ is independent of $V_{\text{imp}}$. In this limit, the pair-breaking effect dominates at all impurity concentrations and $T_c$ is determined by $p_{\text{imp}}$ alone.

In conclusion, we have shown how atomic-scale disorder generates highly inhomogeneous effective pairing interactions within a spin-fluctuation pairing scenario. This results in a superconducting phase with local regions of large gap enhancements compared to the homogeneous system, and makes the superconductor much more robust to disorder, in some cases enhancing $T_c$ of the disordered system. The mechanism described in this work is enhanced for larger impurity potentials, and by the proximity of the system to a magnetic instability. It is a likely explanation for the well-known slower decrease of $T_c$ with disorder in cuprates relative to that anticipated from AG theory [3–7], and may also be related to a recently observed increase of $T_c$ with electron irradiation in FeSe [33].

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