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.

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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 unconventionally paired systems, 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 has 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

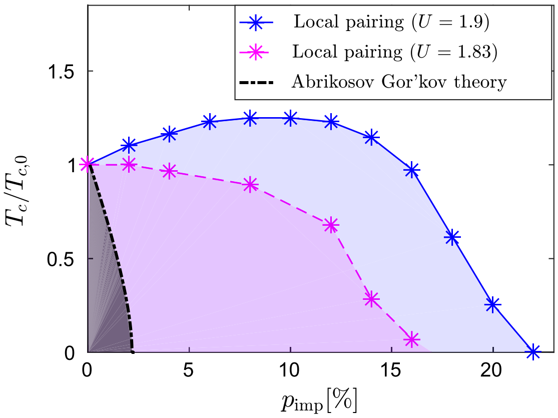

FIG. 1. Critical superconducting transition temperature T_c as a function of disorder concentration for nonmagnetic impurities of strength $V_{\rm imp} = 2$ in d-wave superconductors of Coulomb interaction strength $U = 1.9$ (blue curve) and $U = 1.83$ (magenta curve). Results are averaged over four different impurity configurations. The black line shows the Abrikosov-Gorkov result corresponding to the $U = 1.9$ case.

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 $p_{\rm imp}$, 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 $p_{\rm imp}$, 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

$$H = -\sum_{i,j,\sigma} t_{i,j} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i\sigma} U n_{i\sigma} n_{i\bar{\sigma}} - \sum_{i\sigma} \mu n_{i\sigma} + \sum_{i,i_{\rm imp},\sigma} V_{\rm imp} \delta_{i,i_{\rm imp}} n_{i\sigma}, \quad (1)$$

with a concentration $p_{\rm imp}$ of nonmagnetic impurities of strength $V_{\rm imp}$ at random sites placed at positions $i_{\rm imp}$. The operator $c^\dagger_{i\sigma}$ refers to creation of an electron with spin σ at lattice site i, and $n_{i\sigma}$ is the number operator of spin σ 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

$$H_0 = -\sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i\sigma} (U\langle n_{i\sigma}\rangle - \mu) n_{i\bar{\sigma}} + \sum_{i,i_{\rm imp},\sigma} V_{\rm imp} \delta_{i,i_{\rm imp}} n_{i\sigma}, \quad (2)$$

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]

$$V^{\rm eff}_{ij} = U + \frac{U^3 \chi_0^2}{\hat{1} - U^2 \chi_0^2}\bigg|_{(i,j)} + \frac{U^2 \chi_0}{\hat{1} - U\chi_0}\bigg|_{(i,j)}. \quad (3)$$

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

$$\chi^{\sigma\sigma'}_{ij} = \sum_{m,n} u_{mi\sigma} u_{mj\sigma} u_{nj\sigma'} u_{ni\sigma'} \frac{f(E_{m\sigma}) - f(E_{n\sigma'})}{E_{n\sigma'} - E_{m\sigma} + i\eta}, \quad (4)$$

in terms of the eigenvectors $u_{m\sigma}$ and eigenvalues $E_{m\sigma}$ of Eq. (2). Thus, $u_{mi\sigma}$ 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 Δ^s_{ij} are calculated via a second self-consistency loop from the full mean-field Hamiltonian given by

$$H_{\rm SC} = H_0 + \sum_{i,j} (\Delta^s_{ij} c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} + \text{H.c.}). \quad (5)$$

In the calculation of the singlet gaps,

$$\Delta^s_{ij} = -\frac{V^{\rm eff}_{ij}}{2} \sum_n [u_{ni} v_{nj} + u_{nj} v_{ni}] \tanh(E_n/2T), \quad (6)$$

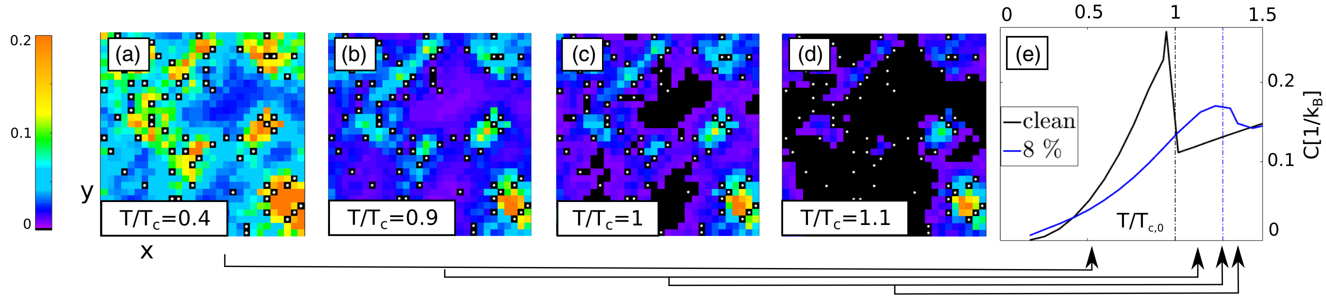

FIG. 2. (a)–(d) Local gap maps below T_c (a),(b), at T_c (c) and above T_c (d) for a system of 8% impurities with $V_{\mathrm{imp}} = 2$. (e) Specific heat as a function of T for the clean system (black line) and for 8% disorder (blue line). The value of T_c as defined by a finite gap exceeding 20% of the homogeneous gap value at $T = 0$ on 60% of the sites is shown by the dashed lines in (e).

we account for superconducting links $\Delta_{i,i+\delta}$, where $\pm\delta \in \{0, \hat{x}, \hat{y}, 2\hat{x}, 2\hat{y}, \hat{x}+\hat{y}, \hat{x}-\hat{y}\}$. $\{E_n, u_n, v_n\}$ are the eigenvalues and eigenvectors resulting from diagonalization of Eq. (5). 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_{imp}. For the results below we fix $U = 1.9$, and explore the dependence of T_c on V_{imp} and p_{imp}.

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

$$\ln\left(\frac{T_c}{T_{c,0}}\right) = \Psi\left(\frac{1}{2}\right) - \Psi\left(\frac{1}{2} + \frac{1}{4\pi T_c \tau}\right). \quad (7)$$

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

$$\frac{1}{\tau} = 2\pi p_{\mathrm{imp}} \frac{V_{\mathrm{imp}}^2 N(0)}{1 + [V_{\mathrm{imp}} N(0)]^2}, \quad (8)$$

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 percolate in the present case of randomly placed pointlike 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], which is not the case here.

Local gap maps at temperatures both below and above T_c are shown in Figs. 2(a)–2(d) for a system with 8% impurities of strength $V_{\mathrm{imp}} = 2$. We show the magnitude of the superconducting d-wave links calculated as $|\Delta_i| = \frac{1}{4}[\Delta_i(\hat{x}) - \Delta_i(\hat{y}) + \Delta_i(-\hat{x}) - \Delta_i(-\hat{y})]$, where $\hat{x}$ ($\hat{y}$) denotes the unit vector along the x axis (y axis). At low T, 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).

Because of 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

$$S = -2\sum_{E_n>0} f(E_n)\ln[f(E_n)] + f(-E_n)\ln[f(-E_n)]. \quad (9)$$

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_{imp} for the case with $V_{\mathrm{imp}} = 2$. 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_{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_{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 $V_{\mathrm{imp}} < 0$ for the cupratelike 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 $\frac{1}{4}[V^{\mathrm{eff}}_{i,i+\hat{x}} + V^{\mathrm{eff}}_{i,i+\hat{y}} + V^{\mathrm{eff}}_{i,i-\hat{x}} + V^{\mathrm{eff}}_{i,i-\hat{y}}]$ for a system of 8% impurities, still with $V_{\mathrm{imp}} = 2$. We calculate the pairing of the dirty system $V^{\mathrm{eff}}(T)$ at $T = 1.2T_{c,0}$, where $T_{c,0}$ is the critical temperature of the clean system and subtract the NN attraction in the pure case $V^{\mathrm{eff}}_0(T_{c,0})$. 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 nonzero 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 Figs. 3(c) and 3(d). For example, a constructive interference of two impurities forming diagonal dimers lead to gap enhancements of ~200% with 6 sites involved, as compared to the ~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.

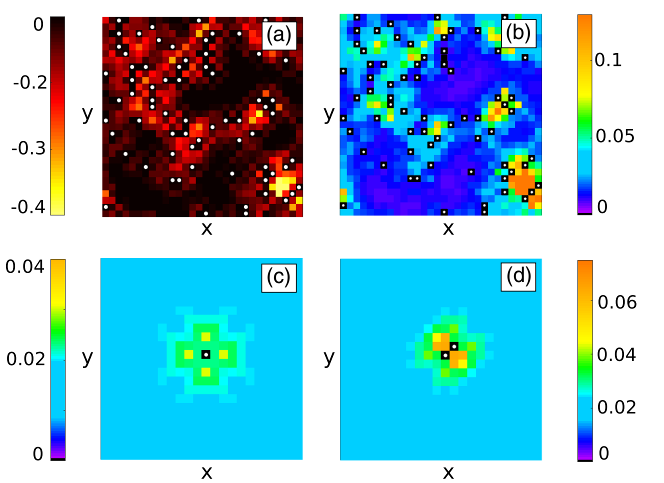

FIG. 3. (a) Real space map of the increase in NN pairing attraction above the pairing strength of the clean system $V^{\mathrm{eff}} - V^{\mathrm{eff}}_0$ at $T = 1.2T_{c,0}$, where $T_{c,0}$ is the critical temperature of the clean system. The system contains 8% impurities of strength $V_{\mathrm{imp}} = 2$ (white dots). (b) The resulting local d-wave gap map for the same system as in (a). Black sites have $\Delta_i < 0.2\Delta(0)$. (c),(d) Local gap at $T = 0.7T_{c,0}$ around a single impurity (c) and two impurities in diagonal-dimer formation (d) of strength $V_{\mathrm{imp}} = 2$. Note the difference in color scale.

In Fig. 4(a) we show the results of the T_c-suppression rate for the case with a weaker impurity potential $V_{\mathrm{imp}} = 1$. As expected, weaker scatterers raise the critical disorder concentration. However, it is found that (i) there remains a substantial difference between the AG result and the local pairing scenario, and (ii) the T_c enhancement is nearly eliminated. There are two reasons for property (i): 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 $\sum_{i\sigma} U\langle n_{i\sigma}\rangle n_{i\bar{\sigma}} = \sum_{i\sigma} U[\Delta n_{i\sigma} n_{i\bar{\sigma}} + (n_0/2)(n_{i\sigma} + n_{i\bar{\sigma}})]$, 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 $\Delta n_{\mathrm{imp}} = \langle n_{\mathrm{imp}}\rangle - n_0 < 0$. This reduces the effective impurity potential $[V_{\mathrm{imp}} + U\Delta n_{\mathrm{imp}}]$, an effect most relevant to weak impurity potentials, and reduces their T_c-suppression rate. The opposite effect happens for magnetic impurities, which

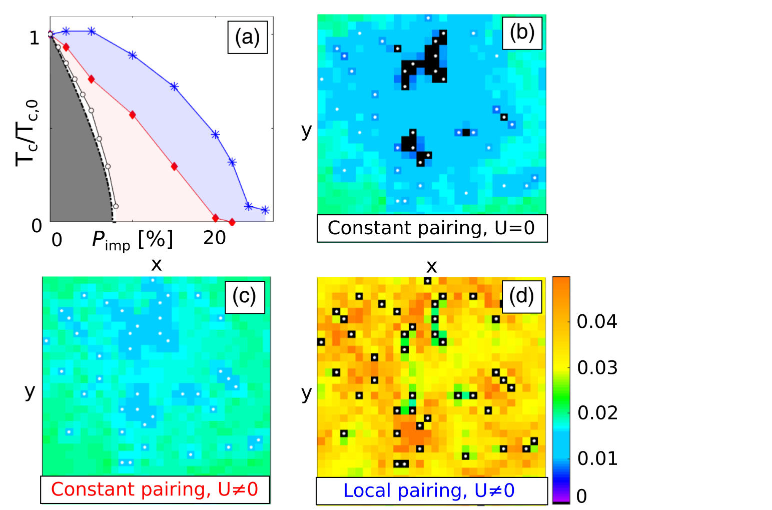

FIG. 4. (a) Suppression of T_c versus nonmagnetic disorder concentration, $V_{\mathrm{imp}} = 1$. The dashed line refers to AG theory. The open circles correspond to a real space calculation with $U = 0$ and constant pairing, roughly confirming the AG result, as expected. The red (blue) curve shows the T_c-suppression for $U = 1.9$, and constant pairing (inhomogeneous local pairing). (b)–(d) Magnitude of the local d-wave gap in a system with 5% disorder at $T = 0.7T_{c,0}$. Impurity positions are marked by white dots. The gap maps correspond to the cases of $U = 0$, constant pairing (b); $U = 1.9$, constant pairing (c); and $U = 1.9$, local pairing (d).

are antiscreened by U [47]. The T_c-suppression rate is further decreased when the electronic correlations are included also in the effective pairing interaction for 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 (ii) above, stronger individual impurities of $V_{\rm imp} \simeq 2$ lead to larger local pairing on neighboring sites compared to $V_{\rm imp} \leq 1$. At small to moderate concentrations $p_{\rm imp}$, stronger impurities are therefore more beneficial for the global T_c. However, a larger impurity potential is more pair breaking, and therefore at large $p_{\rm imp}$ 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 $V_{\rm imp}$ [40]. In this limit, the pair-breaking effect dominates at all impurity concentrations and T_c is determined by $p_{\rm imp}$ 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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