Insensitivity of *d*-wave pairing to disorder in the high-temperature cuprate superconductors

A. F. Kemper,[1,][*] D. G. S. P. Doluweera,[2] T. A. Maier,[3] M. Jarrell,[2] P. J. Hirschfeld,[1] and H-P. Cheng[1]

[1]*Department of Physics, University of Florida, Gainesville, Florida 32611, USA*
[2]*Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221, USA*
[3]*Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

Using a dynamical cluster quantum Monte Carlo approximation, we investigate the effect of local disorder on the stability of *d*-wave superconductivity including the effect of electronic correlations in both particle-particle and particle-hole channels. With increasing impurity potential, we find an initial rise of the critical temperature due to an enhancement of antiferromagnetic spin correlations, followed by a decrease of T_c due to scattering from impurity-induced moments and ordinary pair breaking. We discuss the weak initial dependence of T_c on impurity concentration found in comparison to experiments on cuprates.

I. INTRODUCTION

Disorder is an essential feature of the superconducting cuprates. Crystal growth procedures lead generically to defects such as grain boundaries, atomic site switching, and vacancies. Additional disorder, often in the form of oxygen or other charged defects, is almost always introduced away from the CuO_2 plane upon doping the parent compound from the Mott insulating state. This last type of disorder may be responsible for local nanoscale electronic inhomogeneity in the superconducting state of the cuprate Bi-2212 indicated by scanning tunneling spectroscopy (STS) experiments.[1–4] These experiments show modulations of the local gap near the impurity sites on the order of the correlation length.[5,6] A recent experiment imaging high-energy resonances thought to be the dopant atoms themselves shows a strong positive correlation of the magnitude of the local spectral gap with the locations of the dopants, leading to suggestions that the origin of the observed gap modulations are caused by atomic scale variations in the pairing interaction.[5,6]

When impurities such as Zn and Ni are substituted for Cu in the CuO_2 plane, or planar defects created by electron irradiation, superconductivity is suppressed.[7–10] Because the screened Coulomb potential due to these defects is very short range,[11] such impurities are frequently modeled by pointlike (δ function) scatterers. The expected form for the suppression of superconductivity in the BCS theory of *d*-wave superconductors is then identical to the expression given by Abrikosov and Gor'kov[12] for magnetic impurities in *s*-wave superconductors (see, e.g., Ref. 13). However, experimentally a significantly slower initial slope of the T_c suppression is observed. For example, Tolpygo *et al.*[10] reported a suppression two to three smaller than the Abrikosov-Gor'kov (AG) curve[10] in resistivity measurements of YBCO films. Other unusual deviations from AG behavior have been observed at larger disorder levels; for example, an electron irradiation study[14] on optimally doped YBCO reported a linear behavior in T_c vs resistivity over the entire T_c range.

Theoretically, several possible effects beyond Abrikosov-Gor'kov theory have been explored. A numerical mean-field study of disordered *d*-wave superconductors[15] including the self-consistent suppression of the order parameter around

each impurity site showed deviations from the AG result. Several authors attempted to account for the slowness of the T_c suppression by assuming that the scattering potential of planar impurities was extended, or anisotropic.[16–19] Recently, Graser *et al.*[20] calculated both T_c and the impurity resistivity ρ within a consistent model of extended potential scatterers, and concluded that the unusual T_c vs ρ behavior seen in cuprate experiments should be attributed to strong correlations or strong-coupling corrections to BCS theory. In general, the effect of correlations on the structure and scattering of quasiparticle states in a disordered *d*-wave superconductors is still an open and very important question for cuprates and other unconventional superconductors.

One interesting consequence of disorder in a correlated electron host is impurity-induced magnetism: nuclear-magnetic-resonance measurements indicate the formation of magnetic moments upon chemical substitution of a nonmagnetic impurity for a Cu.[21,22] This was corroborated by calculations of the magnetic spin susceptibility, which displays Curie-Weiss behavior upon impurity doping (see, e.g., Ref. 23). Several aspects of theory and experiment in connection with disorder-induced magnetism in cuprates and one-dimensional (1D) spin systems have recently been reviewed in Ref. 24. While most of the theoretical work on these questions has been confined to the normal state, the quasiparticles deep in the *d*-wave superconducting state are also affected. Mean-field calculations utilizing the Gutzwiller approximation[25] suggest that the effects of disorder on the density of states are suppressed in the presence of strong correlations, specifically near the nodes and at low energies. Similar effects in the density of states are also recovered in calculations where correlations are treated in a simple Hartree-Fock scheme by Andersen *et al.*,[26] who found however that although the effects of disorder on the density of states were indeed weakened, some unusual effects outside the framework of BCS theory were also present, e.g., the breakdown of universal transport in *d*-wave superconductors.[27]

In this paper, we aim to understand some of the effects of disorder on the suppression of the transition to *d*-wave superconductivity. First, a small concentration of weak impurities is shown to cause an increase in the effective antiferromagnetic exchange coupling, which enhances

superconductivity within the Hubbard model. At the same time, the disorder causes pair breaking, which tends to suppress T_c. As the impurity potential is increased, the pair breaking overcomes the enhancement of J causing a decrease in T_c, which continues until it saturates when the unitary limit is achieved. We suggest that these effects may partially account for the observed slow suppression of T_c by disorder in the cuprates.

II. FORMALISM

The Hamiltonian of our model is

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\sigma} n_{i-\sigma} + \sum_i V_i n_{i\sigma}, \quad (1)$$

where $c_{i\sigma}^{\dagger}(c_{i\sigma})$ creates (destroys) an electron with spin σ at site i, and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. Here $\langle ij \rangle$ denotes nearest-neighbor sites i and j, U denotes the on-site Coulomb repulsion, and t is the nearest-neighbor hopping amplitude. The impurity is modeled as a potential $V_i = V$ on a single site. We shall give a brief review of the method (see Ref. 23 for further details).

To study Eq. (1), we employ the dynamical cluster approximation (DCA).[28–30] The DCA is a dynamical mean-field theory which self-consistently calculates the self-energy on a cluster of size N_c embedded in a host. Correlations on the cluster are treated explicitly. Interactions beyond the cluster scale are dealt with on a mean-field level within the self-consistent host. With increasing cluster size, the DCA systematically interpolates between the single-site dynamical mean-field theory (DMFT) (Ref. 31) and the exact result. Cluster dynamical mean-field calculations (including the DCA) of the Hubbard model are found to correctly obtain many of the features of the cuprates, including a Mott gap and strong AF correlations, d-wave superconductivity and pseudogap behavior.[30] To solve the cluster problem, we use a quantum Monte Carlo (QMC) algorithm,[32] and employ the maximum entropy method[33] to calculate the real frequency dynamic spin susceptibility. The sign problem in QMC is small for the values of U considered, and is therefore not an issue for the calculations presented here.

The result of the QMC calculation depends on the disorder configuration, but T_c is determined by the average Green's function, which we compute in the following way. For a concentration x, contributions with m impurities on the cluster are weighted by a combinatoric factor $x^m(1-x)^{N_c-m}$. It is reasonable, for small concentrations ($x < 1/N_c$), to consider only those configurations with zero or one impurities. For the zero and one impurity case, the combinatoric factors expand to $1 - xN_c$ and xN_c, respectively. We can then write the disorder average,

$$G_{ij}^c = xN_c G_{1,ij}^c + (1 - xN_c)G_{0,ij}^c, \quad (2)$$

where $G_{m,ij}^c$ is the cluster real-space Green's function for m impurities. The disorder-averaged Green's function is then used to continue the DCA algorithm.

To determine the critical temperature T_c, we extrapolate the pair-field susceptibility $\chi_d(T)$,[30] and note that the system enters the superconducting state when $\chi_d(T)$ diverges. To interpret the results we present below, we will also need to
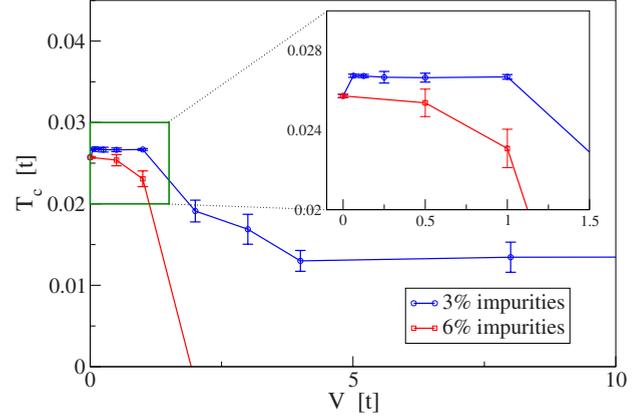
FIG. 1. (Color online) The critical temperature T_c as a function of impurity potential for $N_c = 16$ and $U = 4t$, at impurity concentrations $x = 3\%$ and $x = 6\%$. Error bars are calculated from the extrapolation of the pair-field susceptibility (Ref. 23). Inset: blowup of the region of small impurity potential.

calculate the induced magnetic moment m. This is done using a method introduced by Krishna-murthy *et al.*[34] We note that the square magnetic moment in the low-temperature limit is proportional to T times the magnetic susceptibility. To study the effect of the impurity, we subtract the pure susceptibility, and arrive at

$$m_{\text{induced}}^2 \propto T(\chi_1^c - \chi_0^c), \quad (3)$$

where χ_1^c and χ_0^c are the susceptibilities of a cluster with a single impurity and a homogeneous cluster, respectively.

III. RESULT

We carry out DCA/QMC calculations using the $N_c = 16$, type A (Ref. 35) cluster for the Hamiltonian in Eq. (1), fix the doping at 10% and let $U = 4t$. Estimates for T_c have been shown to be robust against cluster size effects.[36] Furthermore, we have investigated a possible finite-size effect by observing the change zero frequency spin-spin correlation function (not shown), which was found not to deviate appreciably from the clean cluster beyond the first nearest neighbor—indicating that the finite-size effect does not play a significant role on the quantities we report.

We first investigate the d-wave superconducting transition temperature T_c and the induced moment of the system as a function of impurity potential V for various values of the impurity concentration.

Our first significant finding is the initial weak increase in T_c in the region $0 < V \leq t$ for 3% impurity concentration (Fig. 1). This is completely unexpected from the point of view of AG theory, where any concentration of impurities of any strength will suppress T_c initially. The increase in T_c with respect to the homogeneous system is slightly less than 4%. After we increase V to a significantly larger value, for example 20t, the d-wave superconductivity still survives and the critical temperature saturates. This is consistent with the BCS theory of pair breaking by pointlike impurities of a d-wave superconductor (without correlations in the particle-
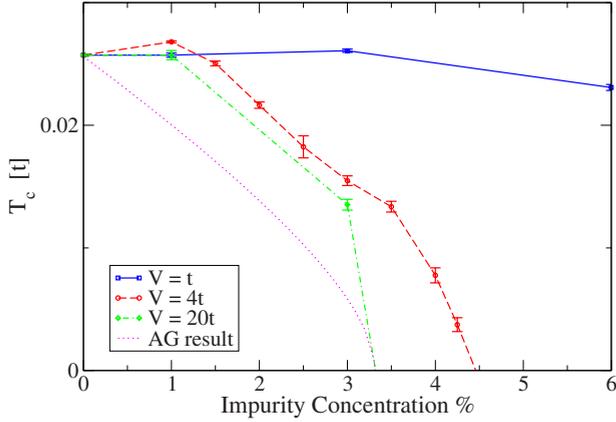
FIG. 2. (Color online) The critical temperature T_c as a function of impurity concentration for $N_c = 16$, and $U = 4t$, at impurity potentials $V = t$, $V = 4t$, and $V = 20t$. Error bars are calculated from the extrapolation of the pair-field susceptibility (Ref. 23). The AG result is a fit to the critical concentration for $V = 20t$.

hole channel), where increasing impurity potential past the bandwidth ($\sim 4t$) drives the impurity into the unitarity limit where the scattering rate saturates.[37] Increasing the impurity concentration beyond 3% causes a dramatic monotonic drop in T_c for all $V > 0$. For 6% impurity concentration T_c vanishes even before $V = 2t$.

Figure 2 shows the behavior of T_c as a function of impurity concentration. For all concentrations considered, the initial slope is either positive or nearly zero, in marked contrast to the Abrikosov–Gor'kov curve, which has a negative initial slope for any combination of impurity concentration and potential. The AG curve plotted was obtained by fitting the unknown parameters to the critical concentration for $V = 20t$, thus forcing the curve to go through the critical concentration calculated by the DCA. While for a given V and impurity concentration we cannot make a direct calculation of the pair breaking parameter entering the noninteracting AG theory and thus determine the critical concentration independently, the qualitative differences of our results from the AG curve shown are obvious, particularly for small concentrations. The critical concentration calculated for strong impurities agrees with the experimentally determined concentration for Cu substitution by magnetic and nonmagnetic impurities in LSCO.[7]

Figure 3 shows the magnetic structure factor $S(\vec{Q}, \omega)$ at $\vec{Q} = (0, \pi)$ of the system at temperature $T = 0.087t$ ($\approx 3T_c$). In analogy with linear spin-wave theory,[38] we note that the peak position of $S(\vec{Q}, \omega)$ at $\vec{Q} = (0, \pi)$ is a measure of the effective exchange coupling $2J_{\text{eff}}$ of the system. Therefore, we use $S[\vec{Q} = (0, \pi), \omega]$ to extract J_{eff} of both ordered and disordered systems. We find that the rise of T_c at low V is correlated with J_{eff} of the system, as shown in the inset of Fig. 3. The initial rise of T_c tracks the initial increase in J_{eff}. Then both T_c and J_{eff} remain nearly constant up to $V = t$. Further increase in V causes J_{eff} to remain roughly constant while T_c shows a dramatic drop, indicating that the suppression at higher concentrations is indeed due to pair breaking rather than pair weakening.
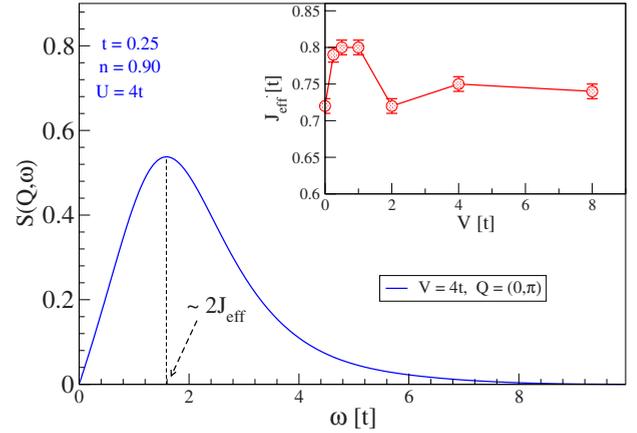
FIG. 3. (Color online) The dynamic spin susceptibility at $\vec{Q} = (0, \pi)$ for $N_c = 16$, $U = 4t$, and $V = 4t$, at impurity concentration $x = 3\%$. The location of the peak, is a measure of the effective spin-wave exchange $2J_{\text{eff}}$ (Ref. 38). Inset: spin coupling constant J as a function of V.

For 3% impurity concentration, T_c starts to drop at $V \simeq U/2$, which is coincident with the formation of impurity-induced moments as shown in Fig. 4. A weak impurity does not induce any local moment in the system and increased J_{eff} causes a rise in T_c; increasing V causes formation of local moments and thereby enhanced pair breaking.

IV. DISCUSSION

Potential scattering due to weak local impurities is expected to inhibit superconductivity because the resulting isotropic scattering in momentum space causes d-wave pair breaking and thus a reduction in the d-wave order parameter. However, the suppression found here is in general weaker than expected from pair breaking due to pointlike potential scatterers in a d-wave system, which follows the AG form. Our results suggest that the slowness of the initial T_c suppression is due to the initial enhancement of the interaction
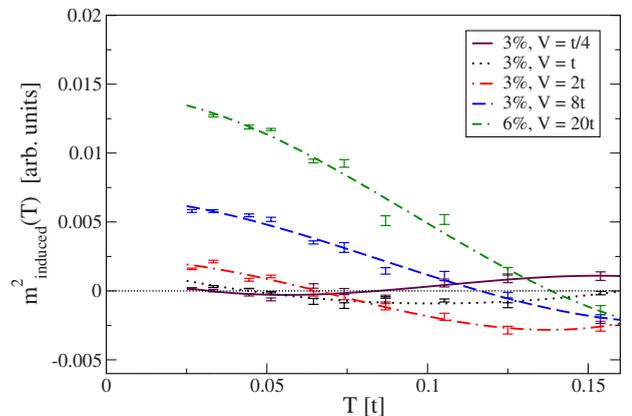
FIG. 4. (Color online) Squared local magnetization [see Eq. (3)] for $N_c = 16$, and $U = 4t$, as a function of temperature for various impurity potentials and concentrations. The solid lines are guides to the eyes.

by the impurities. These results are consistent with recent calculations[39] where the authors argue that an isolated impurity in a *t-J* model can enhance pairing locally. Since the instantaneous part of the pairing potential in the *t-J* model is proportional to J,[40] the local pairing and the transition temperature T_c are enhanced. Here we have confirmed that for impurities, T_c rises along with J. Intuitively, the increase in J can be understood by considering the second-order exchange between two spins on sites with unequal energies, as discussed in Ref. 39.

We are not aware of any experimental data indicating an actual increase or complete insensitivity of T_c to increasing weak disorder in the cuprates, when doping is held fixed. It is not surprising, however, that our results overestimate the pairing enhancement effect of disorder, given the crude way in which disorder averaging has been performed here due to the current limitations on cluster size. Nevertheless, we regard these results as a strong indication that the observed slow initial suppression of T_c in the cuprates, which has been remarked upon for many years, has its origin in large part in correlation effects. A point in the same general spirit was made within a different scheme for treating interactions in Ref. 18.

V. CONCLUSIONS

We have studied the effect of pointlike impurities in cuprates using the dynamical cluster approximation. Our results show that for weak local impurities, the superconducting critical temperature T_c is weakly increased due to an average, impurity-induced enhancement of the antiferromagnetic exchange correlation J. With increasing impurity strength, local moments start to form around the impurity site, causing more quasiparticle scattering, and the critical temperature plateaus subsequently decreases due to pair breaking in both potential and magnetic channels. The suppression of T_c continues until the unitary scattering limit is reached, and T_c remains constant.

As a function of impurity concentration, T_c is found to be enhanced by or insensitive to small amounts of disorder, and although with large disorder T_c is driven to zero, the suppression appears to be generally weaker than that predicted in Abrikosov-Gor'kov theory, where the slope of T_c versus impurity concentration and potential is negative for all concentrations and potentials larger than zero. Our results therefore strongly suggest that the observed slow suppression of T_c is related to the strong correlations in the system neglected in the BCS approach to disorder in a *d*-wave superconductor. Together with the results of Garg *et al.*[25] and Andersen *et al.*,[26] our work suggests a robustness of superconductivity in the presence of correlations against weak disorder in the charge channel.

*kemper@qtp.ufl.edu

[1] T. Cren, D. Roditchev, W. Sacks, J. Klein, J.-B. Moussy, C. Deville-Cavellin, and M. Laguës, Phys. Rev. Lett. **84**, 147 (2000).

[2] C. Howald, P. Fournier, and A. Kapitulnik, Phys. Rev. B **64**, 100504(R) (2001).

[3] S. H. Pan *et al.*, Nature (London) **413**, 282 (2001).

[4] K. M. Lang, V. Madhavan, J. E. Hoffman, E. W. Hudson, H. Eisaki, S. Uchida, and J. C. Davis, Nature (London) **415**, 412 (2002)

[5] T. S. Nunner, B. M. Andersen, A. Melikyan, and P. J. Hirschfeld, Phys. Rev. Lett. **95**, 177003 (2005).

[6] T. S. Nunner, W. Chen, B. M. Andersen, A. Melikyan, and P. J. Hirschfeld, Phys. Rev. B **73**, 104511 (2006).

[7] G. Xiao, M. Z. Cieplak, J. Q. Xiao, and C. L. Chien, Phys. Rev. B **42**, 8752 (1990).

[8] T. R. Chien, Z. Z. Wang, and N. P. Ong, Phys. Rev. Lett. **67**, 2088 (1991).

[9] F. Rullier-Albenque, P. A. Vieillefond, H. Alloul, A. W. Tyler, P. Lejay, and J. F. Marucco, Europhys. Lett. **50**, 81 (2000).

[10] S. K. Tolpygo, J.-Y. Lin, M. Gurvitch, S. Y. Hou, and J. M. Phillips, Phys. Rev. B **53**, 12454 (1996).

[11] L.-L. Wang, P. J. Hirschfeld, and H.-P. Cheng, Phys. Rev. B **72**, 224516 (2005).

[12] A. Abrikosov and L. Gor'kov, Zh. Eksp. Teor. Fiz. **39**, 1781 (1960).

[13] A. Balatsky, I. Vekhter, and J.-X. Zhu, Rev. Mod. Phys. **78**, 373 (2006).

[14] F. Rullier-Albenque, H. Alloul, and R. Tourbot, Phys. Rev. Lett. **91**, 047001 (2003).

[15] M. Franz, C. Kallin, A. J. Berlinsky, and M. I. Salkola, Phys. Rev. B **56**, 7882 (1997).

[16] G. Haran and A. D. S. Nagi, Phys. Rev. B **54**, 15463 (1996).

[17] G. Haran and A. D. S. Nagi, Phys. Rev. B **58**, 12441 (1998).

[18] M. L. Kulic and V. Oudovenko, Solid State Commun. **104**, 375 (1997).

[19] M. L. Kulic and O. V. Dolgov, Phys. Rev. B **60**, 13062 (1999).

[20] S. Graser, P. J. Hirschfeld, L.-Y. Zhu, and T. Dahm, Phys. Rev. B **76**, 054516 (2007).

[21] H. Alloul, P. Mendels, H. Casalta, J. F. Marucco, and J. Arabski, Phys. Rev. Lett. **67**, 3140 (1991).

[22] A. V. Mahajan, H. Alloul, G. Collin, and J. F. Marucco, Phys. Rev. Lett. **72**, 3100 (1994).

[23] T. A. Maier and M. Jarrell, Phys. Rev. Lett. **89**, 077001 (2002).

[24] H. Alloul, J. Bobroff, M. Gabay, and P. Hirschfeld, Rev. Mod. Phys. **81**, 45 (2009).

[25] A. Garg, M. Randeria, and N. Trivedi, arXiv:cond-mat/0609666 (unpublished).

[26] B. M. Andersen and P. J. Hirschfeld, Phys. Rev. Lett. **100**, 257003 (2008).

[27] P. A. Lee, Phys. Rev. Lett. **71**, 1887 (1993).

[28] M. H. Hettler, A. N. Tahvildar-Zadeh, M. Jarrell, T. Pruschke, and H. R. Krishnamurthy, Phys. Rev. B **58**, R7475 (1998).

[29] M. H. Hettler, M. Mukherjee, M. Jarrell, and H. R. Krishnamurthy, Phys. Rev. B **61**, 12739 (2000).

[30] T. Maier, M. Jarrell, T. Pruschke, and M. Hettler, Rev. Mod. Phys. **77**, 1027 (2005).

[31] A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).

[32] M. Jarrell, T. Maier, C. Huscroft, and S. Moukouri, Phys. Rev. B **64**, 195130 (2001).

[33] M. Jarrell and J. Gubernatis, Phys. Rep. **269**, 133 (1996).

[34] H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B **21**, 1003 (1980).

[35] D. D. Betts, H. Q. Lin, and J. S. Flynn, Can. J. Phys. **77**, 353 (1999).

[36] T. A. Maier, M. Jarrell, T. C. Schulthess, P. R. C. Kent, and J. B. White, Phys. Rev. Lett. **95**, 237001 (2005).

[37] P. Hirschfeld, D. Vollhardt, and P. Wolfle, Solid State Commun. **59**, 111 (1986).

[38] E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).

[39] M. M. Maśka, Żaneta Śledź, K. Czajka, and M. Mierzejewski, Phys. Rev. Lett. **99**, 147006 (2007).

[40] T. A. Maier, D. Poilblanc, and D. J. Scalapino, Phys. Rev. Lett. **100**, 237001 (2008).