PHYSICAL REVIEW B, VOLUME 63, 020505(R)

Spatial inhomogeneities in disordered *d*-wave superconductors

Amit Ghosal, Mohit Randeria, and Nandini Trivedi
Department of Theoretical Physics, Tata Institute of Fundamental Research, Mumbai 400005, India
(Received 28 April 2000; published 20 December 2000)

We study a short coherence length *d*-wave superconductor with a finite density of unitary scatterers using the Bogoliubov-deGennes technique. We find that the low-energy density of states is reduced, the superfluid stiffness is significantly larger, and off-diagonal long-range order is more robust than the conventional self-consistent *T*-matrix prediction. These results are a consequence of the inhomogeneous pairing amplitude in the ground state and of the low-lying excitations formed by hybridized impurity resonances. This inhomogeneous response accounts for the insensitivity of high-T_c superconductors to impurities.

DOI: 10.1103/PhysRevB.63.020505 PACS number(s): 74.20.Mn, 71.55.Jv, 74.40.+k, 74.62.Dh

One of the important puzzles in high-T_c superconductors (SC) is to understand why these materials are so insensitive to the effects of disorder, despite the fact that conventional theories would suggest that impurities are pair breaking in a *d*-wave SC. In this paper we show that the *inhomogeneous response* of short-coherence length SC to an impurity potential allows the system to maintain long-range phase coherence up to much higher disorder than one would have expected based on conventional *T*-matrix calculations.

Another motivation for the present study comes from recent progress on the understanding of the response of high-T_c superconductors to a single impurity atom. A unitary scatterer was predicted by Balatsky and coworkers[1] to lead to a low-energy resonance with a characteristic fourfold symmetric wave function about the impurity site. This was recently observed in a scanning tunnel microscope (STM) study[2] of a Zn-doped cuprate. The *T*-matrix approximation used in Ref. 1 is adequate for the one-impurity problem, and the order-parameter suppression near the impurity, which it neglects, does not lead to any qualitative changes. On the other hand, the problem of a finite density of unitary scatterers is more subtle.[3]

There is a large body of theoretical work using the self-consistent *T*-matrix approximation leading to very interesting predictions.[4–7] However, the *assumption* of a homogeneous ground state in the disordered SC in this approach, and others[8] that go beyond it, ignores the nontrivial spatial structures that arise in a short coherence length (ξ_0) SC in response to the disorder potential.

We use the Bogoliubov-deGennes (BdG) approach to study these effects, and to understand how they affect the low-energy properties of the system such as the one-particle density of states (DOS) $N(\omega)$ and the superfluid stiffness D_s. Our main results can be summarized as follows: (1) The low-energy DOS is considerably reduced relative to the *T*-matrix result. The low-lying excitations, generated by the interference of individual impurity resonances are found to have nontrivial spatial structure. (2) We find that off-diagonal long-range order (ODLRO) and finite D_s survive to impurity concentrations much higher than the critical concentration of the *T*-matrix approximation. We show how the inhomogeneity of the pairing amplitude on the scale of ξ_0 in response to a random potential is responsible for this relative insensitivity to impurities. In contrast, conventional approaches assume a uniform amplitude which then gets globally suppressed to zero at a critical disorder.

Several authors have previously used the BdG approach for dirty *d*-wave systems. T_c reduction, superfluid density and localization of excitations was studied in Ref. 9 and more recently the density of states has been studied in Refs. 10 and 11. Our calculations differ from these in several aspects: choice of Hamiltonian, parameters, particle-hole asymmetry, working at fixed density rather than fixed chemical potential, and inclusion of inhomogeneous Hartree-Fock shifts. While our results are broadly consistent with those obtained previously, here our emphasis is on understanding the BdG results for $N(\omega)$, D_s, and ODLRO in terms of two different effects: (a) the inhomogeneity in the local pairing amplitude in the disordered ground state, and (b) the spatial structures characterizing the low-lying excitations in the disordered system. This provides a deeper insight into our results.

We model the two-dimensional (2D) disordered *d*-wave SC by the Hamiltonian $\mathcal{H}=\mathcal{K}+\mathcal{H}_{\rm int}+\mathcal{H}_{\rm dis}$. The kinetic energy $\mathcal{K}=-t\Sigma_{\langle ij\rangle,\alpha}(c^\dagger_{i\alpha}c_{j\alpha}+\text{H.c.})$ describes electrons, with spin α at site i created by $c^\dagger_{i\alpha}$, hopping between nearest neighbors $\langle ij\rangle$ on a square lattice. The interaction term[12] $\mathcal{H}_{\rm int}=J\Sigma_{\langle ij\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-n_in_j/4)+U\Sigma_i n_{i\uparrow}n_{i\downarrow}$ is chosen to lead to a *d*-wave SC ground state in the disorder-free system. The spin operator $S^a_i=c^\dagger_{i\alpha}\sigma^a_{\alpha\beta}c_{i\beta}$, where the σ^a are Pauli matrices, and the density $n_{i\alpha}=c^\dagger_{i\alpha}c_{i\alpha}$ with $n_i=n_{i\uparrow}+n_{i\downarrow}$. Finally, $\mathcal{H}_{\rm dis}=\Sigma_i[V(i)-\mu]n_i$ where μ is the chemical potential and the disorder potential $V(i)$ is an independent random variable at each site which is either $+V_0$, with a probability $n_{\rm imp}$ (impurity concentration), or zero. We believe that such a simple model is adequate to describe the strongly-correlated cuprates at low temperatures because their SC state has sharp quasiparticle excitations.

The BdG equations are given by

$$\begin{pmatrix} \hat{\xi} & \hat{\Delta} \\ \hat{\Delta}^* & -\hat{\xi}^* \end{pmatrix}\begin{pmatrix} u_n \\ v_n \end{pmatrix}=E_n\begin{pmatrix} u_n \\ v_n \end{pmatrix}, \tag{1}$$

where $\hat{\xi}u_n(j)=-\Sigma_\delta(t+W_j)u_n(j+\delta)+[V(j)-\tilde{\mu}_j]u_n(j)$ and $\hat{\Delta}u_n(j)=\Sigma_\delta\Delta(j+\delta;\delta)u_n(j+\delta)$, and similarly for $v_n(j)$. The pairing amplitude on a bond $(j;\delta)$, where $\delta=\pm\hat{\mathbf{x}},\pm\hat{\mathbf{y}}$, is defined by $\Delta(j;\delta)=-J\langle c_{j+\delta\downarrow}c_{j\uparrow}$

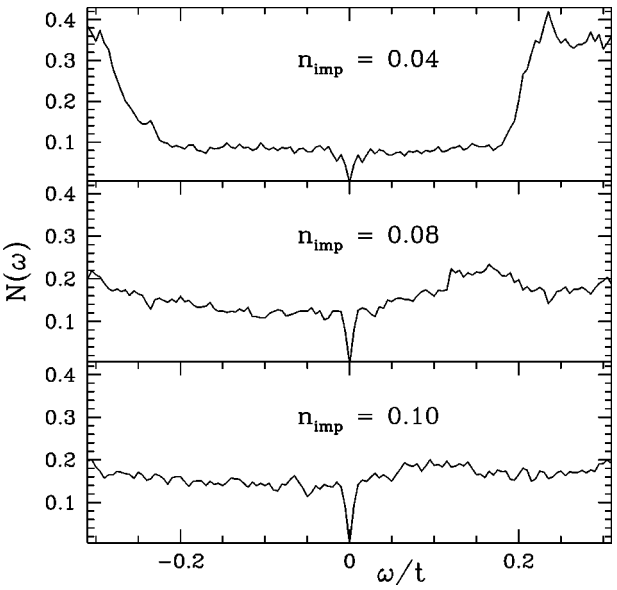

FIG. 1. Density of states (DOS) on a $N=24\times 24$ system, with $J=U=1.15t$ and $\langle n\rangle=0.875$, averaged over 40 disorder realizations at each $n_{\rm imp}$. Note the sharp drop in the DOS near $\omega=0$ on a scale much smaller than the energy gap of $0.31t$ in the pure system.

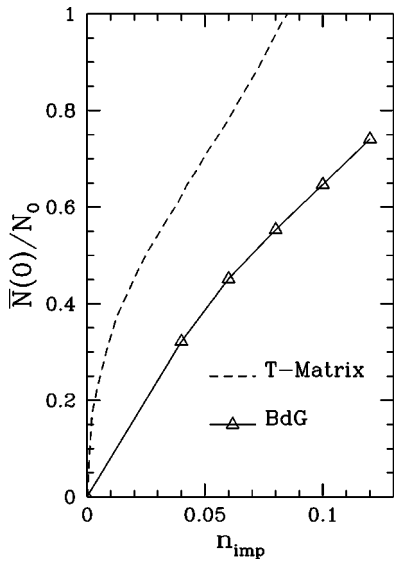

FIG. 2. BdG density of states (DOS) $\bar{N}(0)$, defined as the average of $N(\omega)$ over the range $|\omega|\leqslant 0.05$, is much smaller than the corresponding T-matrix result. The parameters are the same as in Fig. 1 and the normalizing factor is the pure system DOS $N_0=0.21$.

$+c_{j\downarrow}c_{j+\delta\uparrow}\rangle/2$. The inhomogeneous Hartree-Fock shifts are given by $\tilde{\mu}_j=\mu-U\langle n_j\rangle/2+J/4\Sigma_\delta\langle n_{j+\delta}\rangle$ and $W_j=J/2\langle c^\dagger_{j,-\alpha}c_{j+\delta,-\alpha}\rangle$.

We numerically solve for the BdG eigenvalues $E_n\geqslant 0$ and eigenvectors (u_n,v_n) on a lattice of N sites with periodic boundary conditions. We then calculate the pairing amplitude $\Delta(j;\delta)=J\Sigma_n[u_n(j+\delta)v_n^*(j)+u_n(j)v_n^*(j+\delta)]/2$ at $T=0$, the density $\langle n_j\rangle=2\Sigma_n|v_n(j)|^2$, and Fock shift $W_j=J\Sigma_n v_n(j+\delta)v_n^*(j)$. These are fed back into the BdG equation, and the process iterated until self-consistency[14] is achieved for *each* of the (local) variables defined on the sites and bonds of the lattice. The chemical potential μ is chosen to obtain a given average density $\langle n\rangle=\Sigma_i\langle n_i\rangle/N$, and the d-wave pairing amplitude is given by $\Delta(j)=[\Delta(j;+\hat{x})-\Delta(j;+\hat{y})+\Delta(j;-\hat{x})-\Delta(j;-\hat{y})]/4$.

We have studied the model for a range of parameters and lattice sizes. Here we focus on $J=U=1.15$, in units of $t=1$, with $\langle n\rangle=0.875$ (similar to the parameters used in Refs. 9 and 13) on systems of size up to 26×26. For these parameters, and $n_{\rm imp}=0$, the noninteracting DOS at the chemical potential $N_0\simeq 0.21$ and $\Delta_0\simeq 0.077$ corresponding to a maximum gap of 0.31. For the impurity potential we choose $V_0=100$, close to the unitary limit. The results are averaged over 15–40 different realizations of the random potential.

Let us first study the DOS $N(\omega)=(1/N)\Sigma_{n,i}[|u_n(i)|^2\delta(\omega-E_n)+|v_n(i)|^2\delta(\omega+E_n)]$ (where we broaden the delta functions with a width comparable to average level spacing). In Fig. 1 we plot $N(\omega)$ for several impurity concentrations on a small energy scale; for comparison, the maximum energy gap in the disorder-free system is 0.31 and the T-matrix self-energy scale[4] $\gamma=\sqrt{n_{\rm imp}\Delta/2N_0}\leqslant 0.25$ for the parameters chosen; (Δ is the T-matrix gap). In the T-matrix theory $N(\omega)$ is a constant for $\omega\leqslant\gamma$, while we find a sharp dip in the DOS close to the chemical potential, consistent with Ref. 11. In fact, we found $N(0)=0$ for *each* impurity configuration at every concentration that we studied. *The scale of the sharp dip at finite $n_{\rm imp}$ was found to be the same as the energy of an isolated impurity resonance.*

It is very clear that the low-energy DOS in the BdG calculations is considerably smaller than that in the T-matrix approximation [even though we do not have the spectral resolution to quantify the asymptotic form of $N(\omega)$ as $\omega\rightarrow 0$]. To highlight this, we compare in Fig. 2 the finite $N(0)$ of the T-matrix analysis[15] with the BdG $\bar{N}(0)$, which is the average of $N(\omega)$ over the (arbitrarily chosen) range $|\omega|\leqslant 0.05\ll\gamma$.

To gain further insight into this difference between the T-matrix and BdG results, we study the wave functions of the low-lying excitations for individual disorder realizations. The probability density $|u_n(i)|^2+|v_n(i)|^2$ corresponding to the lowest-energy states at various impurity concentrations are plotted in the right-hand panels of Fig. 3.

The resonance for a single unitary impurity shows characteristic powerlaw tails along diagonal directions.[1,16] From Fig. 3, and other low-lying excitations not shown here, we see that for finite $n_{\rm imp}$ these wave functions are generated by the hybridization of individual impurity resonances. The effects of constructive and destructive interference between the ''diagonal tails'' of individual resonances are apparent. The importance of such states was suggested in Ref. 3; however, their analysis assumed that the resonance energies are randomly distributed over a scale $W\gg\Delta_0$, which is not the case in the physical situation obtained here.

We emphasize that excitations with such nontrivial spatial structures cannot be described by T-matrix theory, which treats the scattering of quasiparticles in a homogeneous (im-

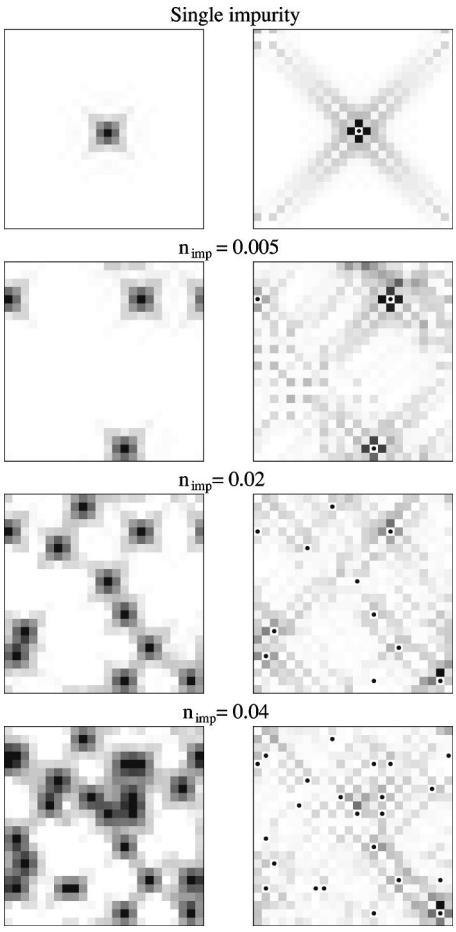

FIG. 3. Left column: Evolution of the local pairing amplitude $\Delta(i)$ with impurity concentration. Dark regions in the gray-scale plot indicate suppressed pairing amplitude, and are correlated with the impurity locations. Parameters used are $J=U=1.15t$ and $\langle n\rangle = 0.875$ on an $N=24\times 24$ system. Right column: The corresponding probability density $|u_n(i)|^2+|v_n(i)|^2$ for the lowest excited state ($n=1$) wave function. Higher probability is indicated by a darker shade. Each impurity location is marked by a dot.

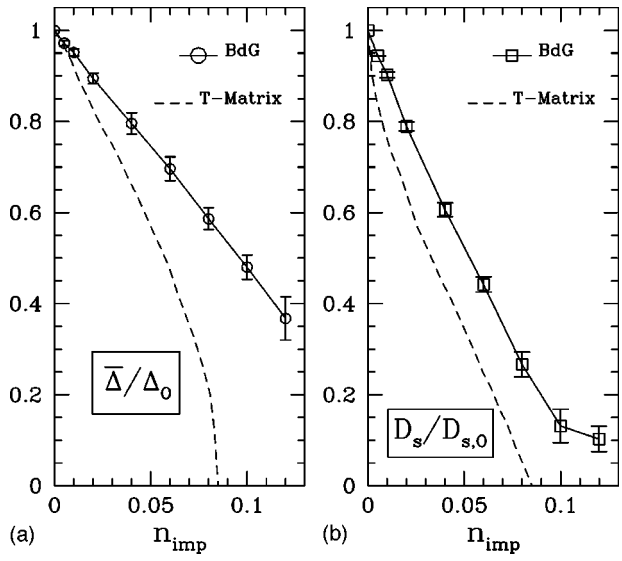

FIG. 4. $T=0$ (a) off-diagonal long-range order parameter and (b) superfluid stiffness (both normalized by their values at zero disorder), as a function of concentration of unitary scatterers, obtained by the BdG method. Note that *d*-wave superconductivity is much more robust than the *T*-matrix prediction. Parameters used are $J=U=1.15t$ and $\langle n\rangle = 0.875$, with $N_0=0.21$ and $D_{s,0}=0.80$, on an $N=24\times 24$ system, averaged over 15 disorder realizations.

purity averaged) medium off a single impurity in a self-consistent fashion. The resulting constant $N(0)$ then arises from a constant broadening γ (defined above) of states near the *d*-wave nodes. In contrast, the low-energy DOS in the BdG theory comes from states arising out of hybridization of impurity resonances.

We already see from Fig. 2 that at and beyond the critical concentration of the *T*-matrix approach, $n_{\rm imp}^c \simeq 0.08$ for our choice of parameters, the BdG DOS does *not* approach the nondisordered value N_0. This raises the questions: does SC persist beyond $n_{\rm imp}^c$, and if so, how? To address these issues we calculate the superfluid stiffness using the linear response result: $D_s/\pi = \langle -k_x\rangle - \Lambda_{xx}(q_x=0, q_y\to 0, \omega=0)$. The diamagnetic term $\langle -k_x\rangle$ is half (in 2D) the kinetic energy $\langle -\mathcal{K}\rangle$, and the paramagnetic term Λ_{xx} is the long wavelength limit of the transverse current-current correlation averaged over disorder realizations.

We see from Fig. 4(b) that the superfluid stiffness D_s is much larger than the *T*-matrix result, consistent with Ref. 9, and does not vanish up to $n_{\rm imp}=0.12$ which is 50% larger than $n_{\rm imp}^c$ within the *T*-matrix approximation. (We did not go to higher impurity concentrations because of the increase in computational time to reach self-consistency.) In any case, we expect that once D_s is sufficiently small, phase fluctuations neglected within the BdG mean-field approach will drive the transition to the nonsuperconducting state;[17] this is left for a future investigation. Here we wish to gain insight into *how* the system manages to exhibit $D_s>0$, even when *T*-matrix theory predicts it to be nonsuperconducting.

One way to think about this is to correlate D_s and $N(\omega)$. A smaller DOS for low-lying excitations in the BdG approach implies fewer ''normal fluid'' excitations and hence a larger superfluid density compared to the *T*-matrix approximation. A complementary approach, which we find very illuminating, relates the D_s to the inhomogeneous pairing amplitude $\Delta(i)$ in the disordered ground state, shown in the left panels of Fig. 3. Notice that the *d*-wave pairing amplitude is suppressed in the vicinity of an impurity on the scale of the coherence length ξ_0 which is 3 to 4 lattice units. (In addition, a small extended *s*-wave component, not shown, also develops nearby). The regions of suppressed pairing amplitude give the appearance of ''swiss cheese''[18] at finite $n_{\rm imp}$ in Fig. 3.

In the *T*-matrix approach the order parameter is forced to be spatially uniform and it vanishes for $n_{\rm imp}\geqslant n_{\rm imp}^c$. However, by allowing the pairing amplitude to vary on the scale of ξ_0, in response to the impurity potential, the BdG solution permits a nonvanishing order parameter $\overline{\Delta}$ which is larger than that obtained within *T*-matrix theory for *all* $n_{\rm imp}$; see Fig. 4(a). ($\overline{\Delta}$ is formally defined in terms of the long distance behavior of the appropriate reduced two-particle density ma-

trix). We note that both $\bar{\Delta}/\Delta_0$ and $D_s/D_{s,0}$ are linear functions of $n_{\rm imp}\xi_0^2$ for a substantial range of impurity concentration.

To qualitatively understand the superfluid stiffness D_s consider applying an external phase twist to the inhomogeneous ground state. Despite the fact that at large $n_{\rm imp}$ there are large regions where the amplitude vanishes, there are still paths that permit phase information to be conveyed from one edge of the system to the other, thus leading to a nonvanishing D_s. Thus the spatial inhomogeneity of the pairing amplitude, which is particularly important in short coherence length superconductors, is crucial in understanding the relative insensitivity of the system to unitary impurities, in that the order parameter and superfluid stiffness are much larger than one might have guessed from the *T*-matrix approximation. This lack of sensitivity of the high-T_c cuprates to disorder has been seen in numerous experiments.[18]

Despite the quantitative results on finite systems and their detailed qualitative understanding, many questions remain open. The first one relates to T_c suppression. While it is easy to calculate the ''mean-field T_c,''[9] a more reliable estimate should include the effect of both phase fluctuations and quasiparticles. Another important question is thermal transport[19] in the SC state. Why does it not reflect the low-energy structure of the DOS and why is it consistent with the universal behavior predicted by *T*-matrix theory,[6,4] when the superfluid density[18] shows deviations from it. A full understanding of the asymptotic DOS of the low-energy excitations, their localization properties and the study of SC state transport on a network of hybridized resonances are all topics for future research.

We would like to thank A.V. Balatsky, P.J. Hirschfeld, A. Paramekanti, S.H. Pan, and G.P. Das for illuminating discussions. M.R. was supported in part by the Department of Science and Technology through the Swarnajayanti scheme.

[1] A. V. Balatsky, M. I. Salkola, and A. Rosengren, Phys. Rev. B **51**, 15 547 (1995); M. I. Salkola, A. V. Balatsky, and D. J. Scalapino, Phys. Rev. Lett. **77**, 1841 (1996).

[2] S. H. Pan *et al.*, Nature (London) **403**, 746 (2000).

[3] A. V. Balatsky and M. I. Salkola, Phys. Rev. Lett. **76**, 2386 (1996).

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

[5] P. J. Hirschfeld and N. Goldenfeld, Phys. Rev. B **48**, 4219 (1993).

[6] M. J. Graf *et al.*, Phys. Rev. B **53**, 15 147 (1996).

[7] K. Maki, in *Lectures on the Physics of Highly Correlated Electron Systems*, AIP Conf. Proc. No. 438, edited by F. Mancini (AIP, New York, 1998).

[8] T. Senthil *et al.*, Phys. Rev. Lett. **81**, 4704 (1998).

[9] M. Franz, C. Kallin, and A. J. Berlinsky, Phys. Rev. B **54**, R6897 (1996); M. Franz *et al.*, *ibid.* **56**, 7882 (1997).

[10] M. E. Flatte and J. M. Byers, Phys. Rev. Lett. **80**, 4546 (1998).

[11] W. A. Atkinson, P. J. Hirschfeld, and A. H. MacDonald, cond-mat/0002333 (unpublished).

[12] The mean-field equations for our model are identical with those of Refs. 9 and 13 *provided* one ignores the Hartree and Fock shifts [defined below Eq. (1)] in all models. However, we choose to work with a *tJ*-like Hamiltonian and keep the appropriate Hartree-Fock shifts.

[13] Y. Wang and A. H. MacDonald, Phys. Rev. B **52**, R3876 (1995).

[14] In order to achieve self-consistency for local pairing amplitudes and Hartree-Fock shifts we had to use the Broyden method [see, e.g., W. E. Pickett, Comput. Phys. Rep. **9**, 115 (1989). The number of iterations necessary to obtain self-consistency grows considerably with disorder; we have checked that the same self-consistent solution is obtained for different initial guesses.

[15] The *T*-matrix results plotted in Figs. 2 and 4 are adapted from Ref. 7 for a particle-hole symmetric, continuum model with the same values of N_0, Δ_0 and $n_{\rm imp}$.

[16] We will discuss elsewhere the dependence of the impurity resonance wave functions on model parameters and on the system size.

[17] A. Ghosal, M. Randeria, and N. Trivedi, Phys. Rev. Lett. **81**, 3940 (1998).

[18] B. Nachumi *et al.*, Phys. Rev. Lett. **77**, 5421 (1996).

[19] L. Taillefer *et al.*, Phys. Rev. Lett. **79**, 483 (1997).