Dopant-modulated pair interaction in cuprate superconductors

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Comparison of recent experimental STM data with single-impurity and many-impurity Bogoliubov-de Gennes calculations strongly suggests that random out-of-plane dopant atoms in cuprates modulate the pair interaction locally. This type of disorder is crucial to understanding the nanoscale electronic structure inhomogeneity observed in BSCCO-2212, and can reproduce observed correlations between the positions of impurity atoms and various aspects of the local density of states such as the gap magnitude and the height of the coherence peaks. Our results imply that each dopant atom modulates the pair interaction on a length scale of order one lattice constant.

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The discovery of nanoscale inhomogeneity in the cuprates has recently generated intense interest. In particular, the spectral gap in the local density of states (LDOS), as observed by scanning tunneling microscopy (STM) [1-4] in Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ (BSCCO), varies by a factor of two over distances of 20-30Å. This unusual behavior may help reveal how the cuprates evolve from the Mott insulating state at half-filling to the superconducting state at finite doping. The hole concentration in the CuO$_2$-planes of BSCCO is proportional to the number of out-of-plane dopant atoms, which also introduce disorder. This has led to the proposition that poorly screened electrostatic potentials of the dopant atoms generate a variation in the local doping concentration and thus give rise to the gap modulations observed in STM [5,6,7]. Poor screening has also been argued to produce enhanced forward scattering [8], which appears to be compatible with photoemission [9,10] and transport measurements [11] in the superconducting state of BSCCO. An alternate perspective is explored in several works which associate inhomogeneous electronic structure with a competing order parameter, such as antiferromagnetism [12,13,14]. Only very recently has it been possible to measure correlations between the inhomogeneities observed in STM and positions of dopant atoms [15], thus providing a clue to the relation between disorder and doping in this compound, as well as a means to examine the above proposals.

In this Letter, we assume that the electronic inhomogeneity observed by STM, at least in the optimally to overdoped samples, can be understood within the framework of BCS theory in the presence of disorder. We show, however, that the conventional modeling of disorder as described above: (i) the subgap spectra are spatially extremely homogeneous, unless they are taken in the immediate vicinity of a defect in the CuO$_2$ plane, (ii) the coherence peaks in regions with larger gap tend to be much broader and reduced in height, (iii) the “coherence peak” positions are symmetric about zero bias, (iv) the dopants are found to correlate positively with large gap regions, and (v) charge modulations are small. We propose that the dopant atoms modulate the local pair potential, i.e. the local attractive coupling $g$ between electrons is spatially dependent. In conventional superconductors, such effects are difficult to observe because atomic-scale modulations in $g$ produce LDOS modulations only on the scale of the coherence length $\xi_0$. In the cuprates, however, the situation is different due to the short coherence length. We demonstrate that a model in which dopant atoms modulate the pair interaction gives excellent agreement with respect to the above mentioned key characteristics of the STM data. A modulated pair interaction could arise from local lattice distortions surrounding the dopant atoms modifying the electron-phonon coupling or superexchange interaction in their vicinity.

Model. We consider the following mean-field Hamiltonian for a singlet $d$-wave superconductor

$$\hat{H} = \sum_{k\sigma} \epsilon_k \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} + \sum_{ij} \sum_{\sigma} V_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \sum_{(ij)} \left( \Delta_{ij} \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger + H.c. \right),$$

where $\epsilon_k = -2t'(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$ and $\sum_{(ij)}$ denotes summation over neighboring lattice sites $i$ and $j$. In the remainder of the paper we will set $t'/t = -0.3$ and adjust $\mu$ to model the Fermi surface of BSCCO near optimal doping (for the homogeneous system, $\mu/t=-1.0$). In order to account for disorder in the out-of-plane dopants, which are separated from the CuO$_2$ plane by a distance $z$, we include an impurity potential modeled by $V_i = V_0 \exp(-r_i/\lambda)/r_i$, where $r_i$ is the distance from a dopant atom to the lattice site $i$ in the plane. Distances are measured in units of $\sqrt{2}a$, where $a$ is the Cu-Cu distance. The nearest-neighbor $d$-wave order parameter $\Delta_{ij} = g_{ij} \langle \hat{c}_{i\uparrow} \hat{c}_{j\downarrow} - \hat{c}_{i\downarrow} \hat{c}_{j\uparrow} \rangle$ is determined self-consistently using [4] with $g_{ij} = g + (V_i + V_j)/2$. In traditional BCS theory, $g_{ij} = g$ is spatially uniform, and $\Delta_{ij}$ is only modulated in the vicinity of potential scatterers [16,17]. We will argue that this approach is unable to reproduce observations (i)-(v) outlined above, and that $g_{ij}$ is strongly modified near the dopant atoms.
Smooth potential. If the potential caused by the out-of-plane dopant atoms were very smooth on the scale of $\xi_0$, the local properties of the inhomogeneous system would be determined by the local value of the disorder potential and the local value of the pairing interaction. Therefore one would expect an LDOS which is locally similar to a clean superconductor with renormalized chemical potential $\mu - V_i$ in the case of a smooth potential $V_i$, or with renormalized bond order parameter $\Delta_{ij} + \delta \Delta_{ij}$ for a smooth off-diagonal (OD) potential. In the case of a conventional diagonal potential, a gap size modulation will be induced because the gap is a relatively sensitive function of the local chemical potential, see Fig. 1(a). On the other hand, modulations of this type will inevitably have coherence peak weight-position correlations opposite to experiment, since large gap values in the homogeneous system imply (within BCS theory) that spectral weight removed from low energies is transferred into the coherence peaks (Fig. 1(b)). This effect is further enhanced by the presence of a van-Hove singularity at $\omega_{vH} = \sqrt{(t'/t)^2 + (\Delta_0)^2}$ in the tight-binding model which contributes additional weight to the coherence peaks, in particular for $\mu/t = -1.2$ where it coincides with the gap edge. Here $\Delta_0$ is the bond order parameter in the homogeneous system. A similar although less pronounced positive correlation between coherence peak weight and position arises also for the smooth OD case. Note that throughout this work we neglect inelastic scattering that would broaden the tunneling conductance peaks at large bias but would not change their weight, thus leaving our conclusions unaffected.

Single-impurity scattering. Since a smooth disorder potential cannot reproduce the experimentally observed relation between the weight of the coherence peak and the gap magnitude, we now address the opposite limit, i.e. a very spiky potential caused by a dopant potential with short range on the scale of $\xi_0$. Some insight into this situation can be obtained by analyzing single-impurity scattering processes, which should be dominant for sufficiently short ranged and weak scattering potentials, where interference effects are negligible. For simplicity we assume constant order parameter in the following $T$-matrix analysis and postpone the fully self-consistent treatment to the many impurity case.

Although solving the $T$-matrix equation for the potential scatterer $V_i = V \delta_{ij}$ is straightforward [13], relatively little attention has been paid to the weak to intermediate strength impurity case $V \lesssim t$ because it does not lead to well-defined resonant states inside the gap. Fig. 2(a) shows the LDOS at the impurity site for a weak pointlike potential scatterer. The positions of the coherence peaks are hardly shifted at all, and while the spectral weight of the coherence peaks is modified, this occurs in a distinctly particle-hole asymmetric fashion. This is in striking contrast to the STM spectra, where inhomogeneous but particle-hole symmetric coherence peak modulations are observed. In addition, there is no distinct feature in experiment corresponding to the van Hove features present, as e.g. in Figs. 1(b) and 2(a).

These shortcomings of the conventional potential scattering model can be overcome by considering OD scattering instead. For the sake of clarity, in this paragraph we neglect the diagonal component of the potential. Fig. 2(b) and Fig. 2(c) show the LDOS at the impurity site for a "pointlike" OD scatterer with $\delta \Delta = \Delta_0$ on the four bonds surrounding the impurity site. Dashed line: extended attractive OD scatterer with $\lambda = \pm 1$. (c) Same as (b), with $\delta \Delta = -\Delta_0$.

![FIG. 1: (a) Order parameter $\Delta_0$ for $t'/t = -0.3$ and a constant nearest neighbor attraction of $\eta/t = 1.16$ as a function of chemical potential $\mu$. (b) Local density of states for different $\mu$ using the order parameter displayed in (a).](image1)

![FIG. 2: On-site LDOS for different single-impurity models with $t'/t = -0.3$, $\mu/t = -1$ and $\Delta_0/t = 0.1$. (a) Weak pointlike potential scatterer. (b) Dotted line: attractive "pointlike" OD scatterer with $\delta \Delta = \Delta_0$ on the four bonds surrounding the impurity site. Dashed line: extended attractive OD scatterer with $\lambda = \pm 1$. (c) Same as (b), with $\delta \Delta = -\Delta_0$.](image2)
suppressed near surfaces [19, 20]. For large negative values of $\delta \Delta$, or more extended OD scatterers, the Andreev resonance moves to smaller energies, and its peak height increases. It draws most of its spectral weight from the van Hove singularity at $(\pi, 0)$, which is close to the part of the Fermi-surface with the largest $d$-wave gap, i.e., the part which is most affected by order parameter modulations. Although this indicates that the weight of the resonance depends on band structure, we find that the phenomenon is very robust over a wide range of $t'$ and $\mu$.

Many-impurity results. In order to strengthen our argument for dopant-modulated pairing interaction we now address the effect of self-consistency and interference between many impurities. To this end, we solve self-consistently the Bogoliubov-de Gennes (BdG) equations resulting from Eq. (1), on a $80 \times 80$ lattice rotated by $\pi/4$ compared to the Cu-O bond direction (as in experimental STM maps), i.e., our system contains $2 \times 80^2$ lattice sites in total. Assuming the dopants are interstitial oxygens, each one most likely contributes two holes to the CuO$_2$ plane. We therefore consider a dopant concentration of 7.5% for optimal doping which are distributed randomly in the reservoir layer separated from the CuO$_2$ plane by a distance $z$.

In the limit of a smooth potential (Fig. 3(a)), the many-impurity results agree well with the local $\mu$ picture discussed above. The correlation between the dopant positions and the gap amplitude depends strongly on the size of the potential due to the non-monotonic dependence of $\Delta_0$ on the local $\mu$, as shown in Fig. 1(a). The spatial variation of the gap, however, is not rapid enough to reproduce the grainy gap maps seen experimentally with gap “patches” of typical size 20-30 Å [3]; one is therefore forced to consider “spikier” potentials (Fig. 3(b)). In the weak limit $V \lesssim t$, one recovers the results of the single-impurity case, i.e., the coherence peaks are modulated in a particle-hole asymmetric way. For the stronger spiky potentials required to reproduce the magnitude of the gap modulations observed in STM, subgap states start to form in contradiction with experiment (see 3(b)). Further discrepancies between Figs. 3(a) and 3(b) and the experimental spectra are: i) the LDOS clearly does not exhibit the inverse relation between gap size and coherence peak height; ii) the spectra are quite particle-hole asymmetric (see Fig. 3(b) and high energy regions in Fig. 3(a)); and iii) the sizable potential required to induce gap modulations inevitably leads to large ($O(50\%-100\%)$) local charge modulations. The latter point puts strong constraints on any potential scattering model, since the primary role of the impurity potential is to couple to the density.

A typical LDOS line scan for a many OD impurity calculation is shown in Fig. 3(c). Note that, by construction, this model has homogeneous low-energy LDOS as well as strong correlations between the dopant positions and the local gap values. As in the single impurity case, the line-shape of the LDOS near the gap edge is determined primarily by Andreev scattering. Because the LDOS near the gap edge is reminiscent of a coherence peak, we will simply adopt this terminology, as used in experiment. The dopant atoms inevitably give rise to a conventional potential as well, however; we therefore show in Fig. 3(d) that the qualitative features of OD scattering depicted in Fig. 3(c) survive this scattering. Comparing Figs. 3(a-d), it is evident that the OD LDOS spectra are far more particle-hole symmetric than those with potential disorder, and display the inverse relation between gap magnitude and coherence peak height, as expected from the single-impurity discussion (see Fig. 2). In Fig. 4 we show the associated gap map (a), the coherence peak height map (b), and the charge modulation map (c) for parameters corresponding to Fig. 3(c). Fig. 4(d) displays the correlation functions between the gap map and the dopants, and the gap map and the peak height map [21]. The local pairing modulation shown in Fig. 4 reproduces qualitatively the correct negative correlation between the gap amplitude and the coherence peak height, the positive correlation between dopant atom locations and large gap values, and the relatively small charge modulations observed in experiment [15]. In addition, the spectra ex-

![Fig. 3: LDOS from self-consistent solution of BdG equations, along a straight line for (a) conventional potential with $z = 2$, $\lambda = 2$, $V_0 = 1.5t$; (b) same as (a), but with $z = 0.57$, $\lambda = 0.5$; (c) OD potential with $V_0$ as in (b); and (d), combination of OD potential shown in (c) with conventional potential as in (b) but with $V_0 = 0.6t$. Conventional (OD) potentials are depicted to right of each panel as a thin (thick) line.](image-url)
we emphasize that nodal quasiparticles are very weakly scattered by this potential, and so microwave and thermal transport are probably only minimally influenced by the effects discussed here [11]. This further implies that the elastic contribution to the ARPES spectral peaks near the antinodal and nodal points are determined by completely different scattering processes.

Conclusions. The discovery of nanoscale inhomogeneity in the local electronic structure of BSCCO-2212 [1,2,3-11] has provoked an intense discussion about the origin of this phenomenon in cuprates and related correlated electron materials. In this work, we have offered strong evidence that the inhomogeneity in the coherence peak position is in fact driven by dopant atoms, located away from the CuO$_2$ plane, whose primary effect on one-particle properties is to modulate the local pair interaction. This ansatz allowed us to reproduce, in model single-impurity and many-impurity calculations, most of the important correlations observed in recent STM experiments.

The calculations reported here have been done entirely within a BCS framework, and as such cannot be expected to reproduce certain other correlations, such as the increase of the average gap with underdoping. Nevertheless, we believe that our results represent an important step towards further modeling which may reveal the microscopic nature of the modulated pair interaction.

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[20] Yu.S. Barash, A. A. Svidzinsky, and H. Burkhardt, Phys. Rev. B 55, 15282 (1997).
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$$C_{f,g}(R) \equiv \int d^2r \frac{[f(r) - \langle f \rangle][g(r + R) - \langle g \rangle]}{\sqrt{A_f A_g}},$$
where $A_f \equiv \int d^2r [f(r) - \langle f \rangle]^2$ and $\langle f \rangle$ is the average of $f$.
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