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Signatures of modulated pair interaction in cuprate superconductors

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Abstract

Recent low-temperature scanning tunnelling spectroscopy experiments on the surface of $Bi_2Sr_2CaCu_2O_{8+x}$ have revealed a strong positive correlation between the position of localized resonances at -960 meV identified with interstitial oxygen dopants and the size of the local spectral gap. We review efforts to understand these correlations within a model where the dopants modulate the pair interaction on an atomic scale. We provide further evidence for this model by comparing the correlations between the dopants and the local density of states with experimental results.
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1. Introduction

High-resolution scanning tunnelling (STS) spectroscopy on BSCCO-2212 has provided some of the most provocative data on cuprate superconductors in recent years, including local information on impurity states, charge ordering, quasiparticles in the vortex state, and nanoscale inhomogeneity. In particular the observation of nanoscale inhomogeneity in the electronic structure of BSCCO-2212 has raised great interest due to its possible relevance to understanding how the cuprates evolve from the doped Mott insulator to the superconducting state. Recently, STS provided intriguing results which may bear on this question, by the observation of random localized resonances at a bias of -960 meV which were argued to be states associated with interstitial oxygen atoms [1]. These defects dope the BSCCO-2212 crystals, along with a rather complex mix of other dopants [2]. From these experiments a strong and positive correlation between the magnitude of the gap and the O dopant positions has been inferred by McElroy et al. [1]. This result was unanticipated, since it

had been suggested [3] that each O might overdope the crystal locally by providing two holes, corresponding to a smaller local gap in analogy with the average gap decrease with overdoping known from tunnelling experiments [4]. Additional salient characteristics of the STS-spectra are their remarkable particle-hole symmetry and their homogeneity at low energies.

Nunner et al. [5] subsequently argued that these main characteristics of the STS-spectra cannot be explained by a model where the dopant atoms act simply as potential scatterers. Instead they suggested that the hypothesis of enhanced pairing around each O-dopant can explain the observed correlations, in particular the negative correlation of the coherence peak height with the magnitude of the gap, i.e. the fact that the coherence peaks are suppressed in regions of large gap and enhanced in regions of small gap. The underlying physics within this model is Andreev-scattering of the quasiparticles at order parameter modulations. In regions of suppressed order parameter a new resonance forms below the gap edge [5] which has been used to explain the extremely sharp coherence peaks observed by Fang et al. [6] in small gap regions. In regions of enhanced order parameter exactly the opposite happens and the coherence peaks are strongly suppressed [5]. The

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fact that the scattering mechanism is of Andreev type can also account for the remarkable particle-hole symmetry of the STS-spectra and for the observed homogeneity at low energies since nodal quasiparticles are less affected by order parameter variations than antinodal quasiparticles. In addition, modulation of the charge is found to be quite weak, in agreement with experiment [1]. None of these effects can be found in models of conventional potential disorder.

Further comparison of the pair disorder model with experiment revealed a natural explanation of the relative strengths of the quasiparticle interference peaks observed in Fourier transform scanning tunnelling spectroscopy (FT-STS) [7] and showed that the broadening of thermodynamic transitions induced by the gap modulations observed by STS was compatible with specific heat measurements on BSCCO-2212 [8]. This serves as an additional evidence that the nanoscale inhomogeneity observed by STS is indeed characteristic of the bulk in the BSCCO-2212 system.

The success of this hypothesis raises the question of whether one can learn about the origins of pairing by studying what modulates it directly [9]. If one were to know the changes in electronic structure induced by a dopant or other impurity, and could establish a direct link to the change in the superconducting order parameter, one would have valuable information with which to constrain theories of superconductivity. A possible microscopic origin of the modulated pair interaction might be the distortion of the crystal lattice around each O interstitial. These local lattice distortions might change local electron–phonon interaction matrix elements or modulate the nearest neighbor hopping t and as a consequence the superexchange constant J between nearest neighbor Cu-atoms (in a one-band model e.g. $J = 4t^2/U$). Within a strong-coupling picture one might assume that the pair interaction is provided by the superexchange J and any modulations of J would directly translate into a modulated pair interaction. This scenario has been further worked out by Zhu [10] with results similar to the ones found by Nunner et al. [5].

To understand the detailed changes in electronic structure around a dopant atom, one can perform an ab initio density functional theory (DFT) calculation of the structure with and without the interstitial present. A first attempt of this type for an oxygen interstitial in the BSCCO-2212 system was made by He et al. [11], who found that the lowest energy location for such a dopant was between the BiO and SrO planes. Remarkably enough, the DFT shows the presence of a narrow band of states near −1 eV induced by the dopant oxygen, as observed in experiment [1]. These states have O(dopant)$2p_z$ character, possibly explaining their strong coupling to the STM tip states, but mix with Bi and O(Bi) states as well. With the results of these calculations, one may now attempt to correlate changes in gap observed by STS with changes in fundamental electronic structure parameters like t, t', electron–phonon coupling constants and Madelung energies.

In the remainder of the paper we provide further evidence in favor of the hypothesis that the oxygen dopant atoms modulate the pair interaction locally rather than to act solely as potential scatterers. For this purpose we calculate the correlation between the local density of state (LDOS) and the modulated pair interaction/disorder potential and compare it with experimental results for the correlation of the LDOS with the positions of the oxygen dopant atoms as found by McElroy et al. [1].

2. Models of inhomogeneity

Our calculations are based on the standard mean field Hamiltonian for a singlet d-wave superconductor

$$\widehat{H} = \sum_{ij\sigma}(t_{ij} + \delta_{ij}(V_i - \mu))\hat{c}_{i\sigma}^\dagger\hat{c}_{j\sigma} + \sum_{\langle ij\rangle}(\varDelta_{ij}\hat{c}_{i\uparrow}^\dagger\hat{c}_{j\downarrow}^\dagger + \text{h.c.}), \quad (1)$$

where we keep only nearest t and next-nearest $t' = -0.3t$ neighbor hopping, with $\mu = -t$ to model the Fermi surface of BSCCO near optimal doping. In the following we consider two models of how the oxygen dopant atoms create inhomogeneity in the local electronic structure. In model (i) we follow the conventional assumption that each oxygen dopant acts as a potential scatterer. The sum of all dopants gives rise to a screened Coulomb potential $V_i = V_0 f_i$ at site i where $f_i = \sum_s \exp(-r_{is}/\lambda)/r_{is}$, with r_{is} the distance from dopant s to the lattice site i in the plane, in units of $\sqrt{2}a$, where a is the Cu–Cu distance. The pair interaction g_{ij} which enters the self-consistency condition for the nearest neighbor d-wave order parameter $\varDelta_{ij} = g_{ij}\langle\hat{c}_{i\uparrow}\hat{c}_{j\downarrow} - \hat{c}_{j\downarrow}\hat{c}_{i\uparrow}\rangle$ is assumed constant, i.e. $g_{ij} = g_0$ in model (i). In model (ii) we assume that each oxygen dopant locally modulates the pair interaction, which we model as $g_{ij} = g_0 + \delta g$ $(f_i + f_j)/2$ with f_i as defined above. In model (ii) the oxygen dopants exert no conventional Coulomb potential, i.e., $V_i = 0$. Since potential scattering enters in the τ_3-channel in Nambu notation we will also call model (i) the τ_3-scattering model. Analogously we will term model (ii) the τ_1-scattering model since order parameter variations enter in the τ_1-channel in Nambu notation.

3. Correlation between LDOS and dopants

In Fig. 1 the LDOS is shown for both the τ_1- and the τ_3-scattering model along typical line cuts. The LDOS has been obtained by solving self-consistently the Bogoliubov-de Gennes equations resulting from Eq. (1) on a 80×80 lattice rotated by 45° with respect to the Cu–Cu bonds, i.e., for a system containing $2 \times 80 \times 80$ sites. Panel (a) shows the LDOS for the τ_1-scattering model. In good agreement with experimental STS-data [12], the LDOS along this linecut shows a strong anticorrelation between height of coherence peaks and gap magnitude. Furthermore, the LDOS is quite particle-hole symmetric and fairly homogeneous at small energies, which is also in favorable agreement with experimental findings. Panels (b) and (c) show the LDOS for the τ_3-scattering model in the limit
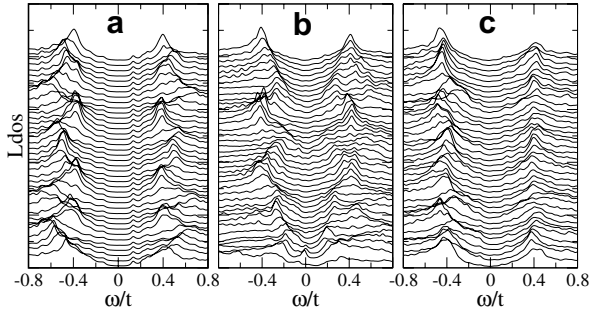
Fig. 1. LDOS along typical line cuts for (a) τ_1-model with $r_z = 0.57$, $\lambda = 0.5$, $\delta g = t$, (b) smooth τ_3-model with $r_z = 2$, $\lambda = 2$, $V_0 = 1.5t$ and (c) "spiky" τ_3-model with $r_z = 0.57$, $\lambda = 0.5$, $V_0 = t$.
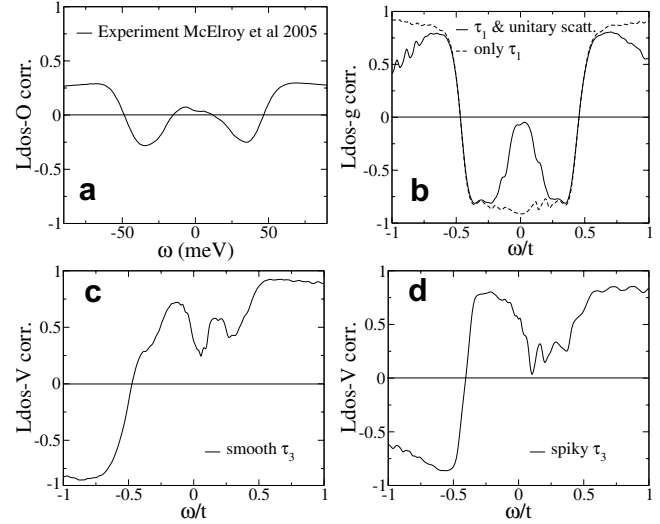

Fig. 2. Correlation function between LDOS and (a) position of the oxygen dopant atoms (experimental) (b) pair interaction $g_i = g_0 + \delta g f_i$ (τ_1-model with $r_z = 0.57$, $\lambda = 0.5$, $\delta g = t$), (c) impurity potential V_i ("smooth" τ_3-model with $r_z = 2$, $\lambda = 2$, $V_0 = 1.5t$) and (d) impurity potential V_i ("spiky" τ_3-model with $r_z = 0.57$, $\lambda = 0.5$, $V_0 = t$).

of a smooth potential variations, which arise if the dopants are poorly screened, and in the limit of a "spiky" potential, which arises when each dopant is well screened and exerts only a short ranged potential. Obviously the τ_3-model fails to reproduce the experimental observations in both limits. In the smooth limit (b) the height of the coherence peaks is positively correlated with the gap magnitude in striking contrast to the experimental observation [1]. In the "spiky" limit (c) gap modulations appear to be quite small, the LDOS lacks particle-hole symmetry and the homogeneity at small energies is destroyed by the formation of sub-gap resonances.

A more direct test for the proposed scattering models is to consider the spatial correlation functions $C_{\rho g}(C_{\rho V})$ between the LDOS $\rho_i(\omega)$ and the modulated pair interaction g_i (impurity potential V_i) which track the O dopant positions in our model. For example, the spatial correlation function between the LDOS $\rho_i(\omega)$ and the impurity potential V_i is defined as

$$C_{\rho V}(\omega) = \frac{\sum_i (\rho_i(\omega) - \langle \rho(\omega) \rangle)(V_i - \langle V \rangle)}{\sqrt{A_\rho A_V}}, \tag{2}$$

where $A_V = \sum_i (V_i - \langle V \rangle)^2$ and $\langle V \rangle$ is the average of V.

The correlation functions for the τ_1- and τ_3-models are shown in Fig. 2 in comparison with the experimental result (panel (a)). The experimental correlation function between the LDOS and the position of the oxygen dopant atoms (a) is remarkably particle-hole symmetric with maximal negative values near ± 35 meV and maximal positive values near ± 70 meV. This behavior of the correlation function reflects the enhancement of the gap close to the oxygen dopant atoms, i.e., the coherence peaks which correspond to additional spectral weight move to higher energies. At small energies the correlation almost disappears, which is a signature of the homogeneity of the LDOS at small frequencies or of the presence of other impurities uncorrelated with the oxygen dopants (see below).

The dashed line in Fig. 2b shows the correlation function $C_{\rho g}$ between the LDOS and the pair interaction $g_i = g_{ii} = g_0 + \delta g f_i$ for the τ_1-scattering model. In good agreement with the experimental curve (a), the correlation function is quite particle-hole symmetric, and is negative

for small energies and positive for large energies. In contradiction to experiment, however, the correlation function remains negative and almost constant at small energies, in particular it does not vanish for energies close to zero. This seems to indicate that the LDOS tracks the local gap magnitude at small energies as one would expect for a smoothly varying pair potential, i.e., the slope of the LDOS at small energies decreases because the gap increases in regions of large pair interaction (close to the oxygen dopants). We believe that this discrepancy with the experimental data is due to the fact that the real BSCCO-2212 system contains further sources of disorder besides the oxygen dopant atoms. In particular, about 0.2% in-plane native defects are typically imaged on a BSCCO-2212 surface. Due to the resonances they generate near zero bias [13] they are generally considered to be strong pointlike scatterers. In order to mimic the real BSCCO-2212 system these additional native defects have to be taken into account.

The solid line in Fig. 2b shows the correlation function $C_{\rho g}$ between the LDOS and the pair interaction for a system where 0.25% strong pointlike potential scatterers ($V = 5t$) have been included in addition to the dopants which only modulate the pair interaction. Obviously, the presence of a small number of unitary scatterers affects the LDOS primarily at very small and at large energies. In particular it destroys the correlation near zero bias. The qualitative agreement between the solid line in panel (b) and the experimental curve in panel (a) is almost perfect. Only the quantitative agreement is not as satisfactory because the correlations in our model calculation are by a factor of 2–3 larger than experimental observations. We speculate that this is due to additional disorder in the real

BSCCO-2212 system which could e.g. stem from the random substitution of Bi at the Sr sites [2].

For comparison the correlation functions $C_{\rho V}$ between the LDOS and the impurity potential V_i for the τ_3-scattering model are shown in Fig. 2c and d in the smooth and "spiky" limit respectively. Both cases are in striking contrast to the experimental data displayed in panel (a). The most drastic discrepancy is the asymmetry of the correlation function in the τ_3-model with respect to zero bias which simply reflects the particle-hole asymmetry of conventional potential scattering and is in clear contradiction to the experimental observation. Only scattering at order parameter variations can account for the remarkable particle-hole symmetry observed experimentally.

4. Conclusions

By comparing the correlation between the LDOS and the oxygen dopants with experimental results we have provided further evidence in favor of a model where the nanoscale inhomogeneity in the local electronic structure of BSCCO-2212 is caused by a dopant modulated pair interaction. Our results demonstrate also that the presence of native defects, which are imaged as scattering resonances near zero bias on typical BSCCO-2212 surfaces, reduces the correlation between the LDOS and the dopant atoms at small energies.

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