Inpurity-induced states in inhomogeneous superconductivity in high-$T_c$ cuprates

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Abstract. Quasiparticle states around a nonmagnetic impurity in inhomogeneous superconducting states observed in high-$T_c$ cuprates are studied using a two-dimensional $t$-$J$ type model. The spatial dependences of the superconducting order parameters are determined within the Bogoliubov-de Gennes theory based on the Gutzwiller approximation. We show that a peak structure is found in the local density of states around the impurity in the large gap regions of the inhomogeneous superconducting states, which has not been experimentally observed yet. Our results suggest that a competing order is realized in the large gap regions in high-$T_c$ cuprates.

1. Introduction

Recent STM/S experiments in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO) have revealed the existence of nanoscale inhomogeneities, that is, a pattern of patches of two different regions with relatively small and large gap[1]. The most prominent features of the inhomogeneities are (i) the pseudogap-phase-like spectra in the large gap regions and (ii) spatially homogeneous subgap spectra both in the small and large gap regions. More recently, it is suggested that out-of-plane disorder, which is inevitably introduced into cuprates to dope charge carriers, is responsible for the inhomogeneity and the gap structures[2]. The inhomogeneity itself generates intense interest in high-$T_c$ physics. Moreover, we expect that observations of inhomogeneity may help reveal unsolved problems in this field for which not even a qualitative theoretical explanation is so far available based on homogeneous theoretical models. Therefore, it is important to investigate the inhomogeneity, especially from the viewpoint of the nature of the large gap region.

To clarify whether the large gap regions have superconducting nature or not, it is helpful to study quasiparticle responses to impurities. Impurity-induced bound states in high-$T_c$ superconductors have been studied extensively [3, 4, 5, 6, 7, 8]. Among various impurities in cuprates, Zn impurities are fundamental perturbations for the ground states because they would be substituted for Cu in the CuO$_2$ plane and then act as nonmagnetic point-like scatterer. The existence of impurity-induced bound states in $d$-wave superconductors was first predicted by Balatsky et al.[3]. Later it has been confirmed in the STS observation on Bi$_2$Sr$_2$Ca(Cu$_{1-x}$Zn$_x$)$_2$O$_{8+\delta}$ (Zn-BSCCO) with high spatial and energy resolution. However, it is reported that no impurity signals are observed in the large gap regions [1].

In this paper, we study the electronic states around the impurity in the large gap regions, assuming that the large gap regions have superconducting nature. We employ two theoretical
models to represent the inhomogeneous superconducting state. One is the patch model recently proposed by Nunner et al. [9], and the other is a random-\(t'\) model, newly introduced here.

2. model

The model we study here is a \(t\)-\(J\) type model with a nonmagnetic impurity at site \(i = 0\), and its Hamiltonian is written as

\[
\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} P_G(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) P_G + \sum_{\langle i,j \rangle} \langle i,j \rangle S_i \cdot S_j
- \sum_{\langle i,j \rangle, \sigma} t_{ij}^p P_G(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) P_G - \mu \sum_{i, \sigma} c_{i\sigma}^\dagger c_{i\sigma} + V_{\text{imp}} \sum_{\sigma} n_{0, \sigma}
\]

(1)

in the standard notation where \(\langle i,j \rangle\) and \((i,j)\) mean the summation over nearest-neighbor and next-nearest-neighbor pairs. The Gutzwiller’s projection operator \(P_G\) is defined as \(P_G = \Pi_i (1 - n_{i\uparrow} n_{i\downarrow})\).

The effects of out-of-plane disorder are introduced to reproduce inhomogeneous superconducting states in two ways: One is a modulation of the superexchange \(J_{ij}\) with a Yukawa form[9]

\[
J_{ij} = J \left(1 + \delta J \frac{r_z}{e^{-r_z/\lambda}}, \frac{e^{-r/\lambda}}{r}\right),
\]

(2)

where

\[r = \sqrt{\left(\frac{r_z + r_i}{2}\right)^2 + r_z^2}.
\]

(3)

Here the region where \(J_{ij}\) is locally enhanced is introduced in the model and we call this region the \(J\)-patch. The other is a random distribution of the values of \(t_{ij}^p\) in the model, keeping the mean value \(\langle t' \rangle\) constant.

The Bogoliubov-de Gennes (BdG) equation based on the Gutzwiller approximation is given as

\[
\left( \begin{array}{cc} H_{ij} & F_{ij}^* \\ F_{ji} & -H_{ji} \end{array} \right) \left( \begin{array}{c} u_{ij}^\sigma \\ v_{ij}^\sigma \end{array} \right) = E^\sigma \left( \begin{array}{c} u_{ij}^\sigma \\ v_{ij}^\sigma \end{array} \right),
\]

(4)

with

\[
H_{ij} = -\sum_{\tau} \left( t_{ij}^{\text{eff}} + t_{ij}^{\text{eff}} \chi_{ij} \right) \delta_{j,i+\tau} - \sum_{\nu} t_{ij}^{\text{eff}} \delta_{j,i+\nu} - \mu \delta_{ij}
\]

\[
F_{ij}^{\ast \sigma} = -\sum_{\tau} J_{ij}^{\text{eff}} \Delta_{ij} \delta_{j,i+\tau},
\]

(5)

where \(i + \tau\) and \(i + \nu\) represent the nearest- and the next-nearest neighbor sites of the site \(i\).

We solve numerically the Bogoliubov-de Gennes equation based on the Gutzwiller approximation and carry out an iteration until the self-consistent equations for order parameters are satisfied. Throughout this paper, we take \(J/t = 0.2\), \(t'/t = -0.3\), \(\delta = 0.15\), \(\delta J = 1\), \(z_0 = \lambda = 1.2[9]\), and \(\langle t' \rangle = -0.3t\).

3. Impurity-induced states in inhomogeneous superconducting states

First, let us look at how the inhomogeneous superconductivity is reproduced by using the \(J\)-patch model or the random-\(t'\) model. Thus we consider here the impurity-free case. Figure 1 (a) shows the local density of states (LDOS) obtained at the center of the \(J\)-patch (the blue line). The LDOS at a site away from the \(J\)-patch is plotted as the black line. We actually see that the
Figure 1. (a) The LDOS at the center of the J-patch (the blue line) and at a site away from the J-patch. (b) Spatial modulation of the LDOS due to the randomness of the next-nearest-neighbor hopping amplitudes $t'_{ij}$.

Coherence peaks are strongly suppressed inside the J-patch, as reported in the previous works [9, 10].

We also show the spatial modulation of the local density of states in the random-$t'$ model in fig. 1 (b). We note here that, in this case, we take $\delta J = 0$, that is, there is no J-patch. It is clear that the prominent features of the inhomogeneity are well reproduced also by using the random-$t'$ model. We find that, since the next-nearest-neighbor term vanishes at the points $(\pm\pi/2, \pm\pi/2)$ in the Brillouin zone, the randomness of $t'_{ij}$ does not affect the spectra near the Fermi energy. This is a reason why the random-$t'$ model can reproduce the inhomogeneity.

Figure 2. (a) The LDOS around the impurity located at the center of the J-patch (the red line). (b) Spatial modulation of the LDOS around the impurity in the random-$t'$ model. The red line shows the LDOS obtained at the nearest-neighbor site of the impurity.

Next, we study the quasiparticle states around the impurity at the center of the J patch, or at the large gap site of the random-$t'$ model. Figure 2 (a) shows the LDOS at the nearest-neighbor site of the impurity (the red line). A fairly large peak structure around the zero-energy is clearly seen in this figure. This is naturally expected from the $d$-wave nature of the superconductivity even in the J-patch. In Fig. 2 (b), we show the spatial variation of the LDOS around the
impurity. We note that these LDOS are plotted along the (10) direction of the square lattice across the impurity, and the red line represents the LDOS at the nearest-neighbor site of the impurity. A peak structure around the zero-energy is also found but in this case there are two peaks in the LDOS around the impurity. The two models employed here have reproduced the inhomogeneity, or the spectra in the large gap regions, assuming that the large gap regions have superconducting nature. Thus, if the large gap regions found in the STM/S experiments are simply superconducting but with larger gap structure, impurity signals should be clearly observed.

4. Summary and Discussion
In this paper, we have shown that the impurity resonance states are clearly seen in the large gap regions of inhomogeneous superconducting states when it has superconducting nature. This result suggests the non-superconducting origin of the large gap regions.

Last, it is worth noting here that quasiparticle resonance states can be induced around a impurity even if the large gap region is not superconducting, as shown by Kruis et al. [6] They have argued that, the mere fact that the LDOS is depleted at the Fermi energy is sufficient to produce resonance states around a nonmagnetic impurity. However, these resonance states would not be observed in tunnel conductance spectra because in such cases, the correspondence between the tunneling conductance and the LDOS would be broke down as shown for the surface states [11].

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References
[1] Lang K M, Madhavan V, Hoffman J E, Hudson E W, Eisaki H, Uchida S and Davis J C 2002 Nature(London) 415 412
[2] McElroy K, Lee J, Slezak J A, Lee D.-H., Eisaki H, Uchida S and Davis J C 2005 Science 309 1048
[3] Balatsky A V, Salkola M I, Rosengren A 1995 Phys. Rev. B 51 15547
[4] Tsuchiura H, Tanaka Y, Ogata M, Kashiwaya S 2000 Phys. Rev. Lett. 84 3165
[5] Pan S H, Hudson E W, Lang K M, Eisaki H, Uchida S and Davis J C 2000 Nature (London) 403 746
[6] Kruis H V, Martin I, Balatsky A V 2001 Phys. Rev. B 64 054501
[7] Balatsky A V, Vekhter I and Zhu J-X 2006 Rev. Mod. Phys. 78 373
[8] Kambara H, Niimi Y, Ishikado M, Uchida S and Fukuyama H 2007 Phys. Rev. B 76 052506
[9] Nunner T S, Andersen B M, Melikyan A and Hirschfeld P J 2005 Phys. Rev. Lett. 95 177003
[10] Fang A C, Capriotti L, Scalapino D J, Kivelson S A, Kaneko N, Greven M, Kapitulnik A 2006 Phys. Rev. Lett. 96 017007
[11] Zhu J-X 2002 Phys. Rev. B 66 104523