The Zinc Doping Induced STM Resonance as a Zero Mode

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Abstract

We show that the Zinc doping induced STM resonance in high-Tc cuprates is a zero mode - a d-wave monomer confined in the opposite sublattice of the Zinc site. We propose that the resonance come from the superconducting peak around $(\pi,0)$ as observed in ARPES experiments. It is predicted that the resonance should vanish in single layer $BSCCO_{2201}$ or in the vortex core of underdoped cuprate where the ARPES peak is absent. We argue that the STM result imply the ARPES peak around $(\pi,0)$ is the only coherent feature in the whole Brillouin zone.
Zinc doping is an important probe of the high temperature superconductors for two reasons. On the one hand, it is a clean probe. The closed shell $Zn^{2+}$ ion substitute for the $Cu^{2+}$ ion in the $CuO_2$ plane and act almost as a vacancy of the lattice and is thus almost parameter free. On the other hand, experiments find dramatic effects of zinc doping in almost all important detecting channels such as transport, spin dynamics and single particle spectrum.

Recently, STM experiments find a sharp resonance near zero energy around the Zinc sites in $BSCCO_{2212}$[1]. Many theoretical efforts have been devoted to extract information from this remarkable phenomena[2, 3, 4, 5, 6, 7]. Roughly speaking, there are two class of theories. The first kind of theory view the resonance as the result of potential scattering of d-wave BCS quasiparticle from the Zinc site. The second kind of theory view the resonance as a result of Kondo effect of the nodal quasiparticle with the presumed Zinc-doping induced local moment. Although experiment result do show some similarity with the prediction of these theories, no theory is truly satisfactory. The following characteristics of the resonance are especially difficult to understand. (1)the resonance is extremely sharp in energy and extremely close to zero energy. (2)the spectral weight of the resonance seems to be transfered totally from the so called coherence peak in the density of state, with other part of the spectrum essentially unchanged(except for a nearly constant downward shift of spectral weight in the particle side). (3)the resonance extend mainly in the antinodal direction rather than the nodal direction in real space. (4)The resonance exist only on the sublattice that the doped Zinc ion resides. Since the observed STM spectrum at any site is actually the sum of spectrums from its four nearest-neighbouring sites(which are on the opposite sublattice of the given site) due to the filtering of the $BiO$ layer intervening the STM needle and the $CuO_2$ plane[7], this indicate that the resonance is confined on the opposite sub-lattice of Zinc site. In the first kind of theory, the resonance mode is well defined only when the system is particle-hole symmetric and the scattering potential is infinite(the resonance energy is zero in this case). However, this symmetry exist only in the half-filled case and is broken in doped system. Many body effect make the situation even worse. For example, STM spectrum shows a large downward slope in the density of state near Fermi level which is attributed to strong correlation effect by some author[8]. The spectral weight transfer pattern and the extending direction of the resonance in real space predicted by these kind of theories are also problematic. Calculation shows the spectrum change on all energy scale
upon Zinc doping even in the particle-hole symmetric case. Correspondingly, the resonance mode always change its extending direction into the nodal direction at large distance since the Fermi velocity is maximum in that direction. For the Kondo-like theories, the most severe problem is that the nature of the presumed local moment and its coupling to the nodal quasiparticle are not clear. At the same time, this mechanism suffers from the same problem as the first kind of theories as regard to the spectral weight transfer pattern and extending direction of the mode in real space since nodal quasiparticle play the central role in this framework. There is also no way to understand the sublattice selection rule in this framework. We note that the Kondo screening vanishes in the particle-hole symmetric case and thus the two kind of interpretations of the resonance are in fact orthogonal.

We take the doped $\text{Zn}^{2+}$ ion as a vacancy of the lattice. We show that the Zinc doping induced single particle resonance is a zero mode confined in the opposite sublattice of the Zinc site. This zero mode is in fact the d-wave partner of the Zinc site whose pairing with the Zinc site is made ineffective by the large potential difference between the two participants of the pairing. Since this is a d-wave state, it spectral weight comes mainly from the antinodal region of the Brillouin Zone and has no contribution from quasiparticle exact along the nodal direction. Guided by this picture, we propose that this resonance comes from the so called superconducting peak near $(\pi, 0)$ observed in ARPES experiments. This proposal has the virtue that the particle-hole symmetry is easily satisfied since the ARPES peak exist only in a small region around $(\pi, 0)$ in which there is almost no dispersion. It also build in naturally the correct spectral weight transfer pattern and correct extending direction of the resonance in real space. This proposition has many interesting predictions. For example, it predicts that the resonance should vanish in vortex core with a pseudogap and in single layer $\text{BSCCO}_{2201}$ where no ARPES peak is observed. This picture also indicated that the ARPES peak around $(\pi, 0)$ is the only coherent spectral feature in the whole Brillouin Zone.

The doped Zinc ion break the translational symmetry of the lattice. However, the point group symmetry with respect to the Zinc site is preserved (here we assume a single Zinc ion for simplicity). Hence we assume that the Zinc doped system preserve the d-wave symmetry of superconducting pairing under the point group operation. With the pairing being d-wave, a s-wave particle can only pair with a d-wave particle and vice versa. Hence the particle
that pair with the Zinc site must be d-wave. Since the kinetic energy of the Hamiltonian is symmetric under the point group operation, such a d-wave particle has no chance to feel the strong s-wave repulsive potential on the Zinc site. Hence the zinc site and its d-wave pairing partner feel a large potential difference due to the symmetry mismatch of pairing and scattering potential. This large potential difference make the pairing ineffective and we simply get a level pushed to large energy and the other essentially unchanged from the its bare energy. In other words, the pairing is broken and we are left with a d-wave particle missing its pairing partner (the missing particle is just the Zinc site). This d-wave monomer, is nothing but the observed resonance in STM spectrum. This picture of the STM resonance as a d-wave monomer naturally explain the fact that the spectral weight of the resonance comes mainly from the antinodal region and that the resonance extend mainly in the antinodal direction. This argument is, however, oversimplified in that we have totally neglected the dispersion caused by the kinetic energy and the pairing potential. With these dispersion present, we generally only get a edge state - a virtual bound state with finite life time and nonzero energy, rather than a well defined mode at zero energy. To show this more directly, we make a T-matrix calculation of the impurity effect in a d-wave BCS state. Here we model the Zinc impurity as a repulsive potential scatter with strength $U$ at the origin. The real space Green’s function is given by

$$g_{i,j} = g^0_{i,j} + g^0_{i,0}U\tau^3[I - g^0_{0,0}U\tau^3]^{-1}g^0_{0,j}$$

here $g^0_{i,j}$ is the Green’s function of the pure system in the Nambu’s notation and is given by the Fourier transform of the momentum space Green’s function, $g^0_{i,j} = \frac{1}{(2\pi)^2} \int d^2k \frac{e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)}}{\omega + i\delta - \xi_k \tau^3 + \Delta_k \tau^1}$

$\tau^1, \tau^3$ are the Pauli matrix appearing in the Nambu notation, $I$ is the identity matrix, $\xi_k$ and $\Delta_k$ are bare dispersion and pairing order parameter. Here we take $\xi_k = -2(\cos(k_x) + \cos(k_y)) - \mu$, $\Delta_k = 2(\cos(k_x) - \cos(k_y))$. In this case, the particle-hole symmetry is explicitly broken by the finite chemical potential at nonzero doping (in general the particle-hole symmetry can also be broken by introducing longer range hopping term that make the lattice non-bipartite). The additional spectral weight caused by Zinc doping come from the pole of the $[I - g^0_{0,0}U\tau^3]^{-1}$. The pole equation has a zero energy solution when the
off-diagonal matrix element of $g_{0,0}^0$ vanish and the system is particle-hole symmetric (which also imply that $U$ is infinite). The first condition correspond to the physical requirement that the pairing partner (not necessarily d-wave) of the Zinc site should have zero amplitude at the origin and so can not feel the strong repulsive potential. The second condition, namely the requirement of particle-hole symmetry, in fact imply that the system is bipartite. To show this, we take a general pairing Hamiltonian on the lattice (not necessarily translational invariant)

$$H = \sum_{i,j,\sigma} t_{i,j} c_{i,\sigma}^\dagger c_{j,\sigma} + \sum_{i,j} (\Delta_{i,j} c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger + h.c.) + \sum_{i,\sigma} \mu_i c_{i,\sigma}^\dagger c_{i,\sigma}$$

$$= H_t + H_\Delta + H_\mu$$

and examine how it transform under the following particle-hole transformation

$$c_{i,\uparrow}^\dagger \longrightarrow c_{i,\downarrow}$$
$$c_{i,\downarrow}^\dagger \longrightarrow c_{i,\uparrow}$$

Under this transformation, the three part of $H$ transform as follow (here we restrict ourself to the case of singlet pairing with a real $\Delta_{i,j}$ for simplicity),

$$H_t \longrightarrow -H_t$$
$$H_\Delta \longrightarrow H_\Delta$$
$$H_\mu \longrightarrow -H_\mu + 2 \sum_i \mu_i$$

For a particle-hole symmetric system, the transformed Hamiltonian should be gauge equivalent to the original one. This requirement has three implications. First, $H_\mu$ should vanish since it is gauge invariant. Second, the lattice should be bipartite in the sense of $H_t$ since otherwise we can always construct a odd-bond loop in which the enclosed flux differ by $\pi$ before and after the transformation. Third, the pairing term should be inter-sublattice only or intra-sublattice only as can be shown by a similar argument provided that the lattice
is connected in the sense of \( H_{ij} \)(that is, any two sites of the lattice can be connected by a path made up of bonds with nonzero \( t_{i,j} \)). For the high temperature superconductors that we are interesting in, the pairing term should be inter-sublattice only for the system to be particle-hole symmetric. Hence the whole Hamiltonian is bipartite(the intra-sublattice pairing case is also bipartite, but in a different sense). For a bipartite system with a vacancy in one sublattice, it is easy to show a mode will appear exactly at zero energy which is confined on the opposite sublattice of the vacancy. The proof of this statement can be briefed as follow. Let \( \psi \) be an eigen mode of the system(i.e. \([\psi, H] = E\psi\)). We can always write \( \psi \) as \( \psi_1 + \psi_2 \), in which \( \psi_1 \) and \( \psi_2 \) denote the components of \( \psi \) in the two sublattices. Since the Hamiltonian is bipartite, we have \([\psi_1, H] = E\psi_2 \) and \([\psi_2, H] = E\psi_1 \). Hence for nonzero \( E \), both \( \psi_1 \) and \( \psi_2 \) are nonzero and \( \psi_1 - \psi_2 \) is a eigen mode of energy \(-E\). At the same time, since \([[\psi_1, H], H] = [\psi_1, H^2] = E^2\psi_1 \) and \([[\psi_2, H], H] = [\psi_2, H^2] = E^2\psi_2 \), \( \psi_1 \) and \( \psi_2 \) are eigen modes of the Hermite operator \( H^2 \) and thus form complete orthogonal basis in the Hilbert space of the two sublattices respectively(for degenerate \( E \), there exist an orthogonal procedure that make each components orthogonal in their respective subspace, the property \( \{\psi_1, \psi^\dagger_1\} = \{\psi_2, \psi^\dagger_2\} \) which follows from the fact that \( \{\psi_1 + \psi_2, \psi^\dagger_1 - \psi^\dagger_2\} = 0 \) is useful in proving this). Thus, nonzero energy eigen mode always appear in pairs and exploit one state from each of the two sublattice. Since the dimension of the Hilbert space of the two sublattice differ by one, there should always be a state on the opposite sublattice of the vacancy that is left unpaired and have zero energy. This mode is in fact a zero mode in general context which exists for topological reason. In our case, the dimension of the Hilbert space of the two sublattices differ by one due to the vacancy. This is analogous to the topological constraint near a domain wall in the 1d Peierls system in which case a zero mode exist \[10\].

The picture of the STM resonance as a d-wave monomer do capture the main characteristics of the experimental result. However, it is still not a interpretation of the experiment until we understand the following points. First, where is the required particle-hole symmetry? As we have mentioned, this symmetry is badly violated in the high temperature superconductors. Second, the d-wave nature of the mode alone is not enough to filter contribution from the nodal region totally. These remaining contribution from the nodal region will dominate the long distance behavior of the mode since the Fermi velocity is maximal in that region and we expect the mode to extend mainly in the nodal direction at sufficient
large distance.

Fortunately, our picture also tell us where to find the way out. Since the spectral weight of the mode is dominated by contribution from the antinodal region, we should focus our attention at this region. Experimentally, ARPES show a characteristic ‘peak-dip-hump’ structure in the antinodal region below the superconducting transition temperature\[9\]. The peak intensity increase with decreasing temperature in a way similar to that of superfluid density. We propose that the Zinc doping induced STM resonance comes from this ARPES peak. This proposition has the virtue that the all important particle-hole symmetry is easily satisfied since the ARPES peak exist only in a small region around \((\pi, 0)\) in which there is almost no dispersion. At the same time, this mechanism also naturally built in the correct spectral weight transfer pattern and the correct extending direction of the mode in real space since it is free from the concomitant of nodal contribution. Since the ARPES peak is dispersionless, we model it as a Fermi surface mode with a d-wave pairing gap of constant amplitude \(\Delta\). In this case, the equation for the pole of \([I - g_{0,0}^0 U^3]^{-1}\) reduce to

\[
\left[1 - U\omega - \frac{\omega}{\omega^2 - \Delta^2}\right] \left[1 + U\omega - \frac{\omega}{\omega^2 - \Delta^2}\right] = 0
\]

here the parameter \(\alpha\) take care of the effect of both wave function renormalization and the vertex renormalization. The solution of this equation is given by

\[
E = \frac{\pm U\alpha \pm \sqrt{(U\alpha)^2 + 4\Delta^2}}{2}
\]

for large \(U\), the solution can be approximated by \(E_1 = \pm U\alpha\) and \(E_2 = \pm \Delta\). The second solution is the zero mode we discussed in this paper. In principle, we can calculate the real space distribution of the mode if we know the momentum distribution of the ARPES peak in the Brillouin Zone. Roughly speaking, the spatial range of the mode in real space is inversely related to the momentum range of the ARPES peak in the Brillouin Zone. The extending direction of the mode in real space is determined by the anisotropy of the momentum region in which the ARPES peak exist. As a simple model, we take the momentum region of the ARPES peak as the rectangular area around \((\pi, 0)\) shown in Figure 1. This assignment is reasonable since the Fermi surface near \((\pi, 0)\) is parallel to the antinodal direction\[9\]. Figure 2 shows the calculated spectrum on the nearest neighbouring site of Zinc, Figure 3 shows the calculated real space distribution of local density of state contributed by the resonance
mode. The results are within our theoretical expectation and consistent with experimental results.

Our proposition for the resonance mode has many interesting predictions. According to our proposition, the STM resonance should vanish with the ARPES peak. We can check this prediction in single layer $BSCCO_{2201}$ since ARPES find no 'peak-dip-hump' structure around $(\pi,0)$ in this material. We can also check the prediction in a magnetic field since it is believed that magnetic field can reduce the intensity of the ARPES peak. Especially, the ARPES peak will vanish totally in a pseudogap phase vortex core and we expect the STM resonance to disappear in the vortex core of a underdoped cuprate.

In our theory, the resonance mode always appear in pairs on both side of bias. For a repulsive scatter, the main spectral weight is particle-like. However, the resonance observed in experiment appear at small negative bias. This means that the resonance mode is occupied by an unpaired electron. This is supported by the nearly constant downward shift of spectral weight in the particle side of the spectrum which imply a local increase of electron density. This conclusion can also be reached by examine the extending direction of the mode in real space since a hole mode should extend mainly in the nodal direction due to the complementary nature particle and hole. According to this picture, we should expect a secondary peak below the main peak which extend mainly in the nodal direction. We note experiments do show a small peak below the main peak. It is interesting to check its extending direction in real space. Mathematically, the ground state of the Zinc-doped system should of the form $\gamma^\dagger_e| paired\rangle$. Here $\gamma^\dagger_e$ is electron-like excitation. The main STM peak should correspond to the process $\gamma^\dagger_e| paired\rangle \rightarrow | paired\rangle$. The secondary peak should correspond to the process $\gamma^\dagger_e| paired\rangle \rightarrow \gamma^\dagger_e\gamma^\dagger_h| paired\rangle$, where $\gamma^\dagger_h$ is a hole-like excitation.

In our discussion, we have neglect the coupling of the ARPES peak with other excitations in the Brillouin Zone. This neglect has important implication. Technically, this coupling can be expressed in terms of the following matrix element

$$\langle \text{ARPES Peak}| \hat{U} | \text{Other excitations} \rangle$$

where $\hat{U}$ is the potential scattering. The vanishing of this coupling indicate that the ARPES peak and other excitations in the Brillouin Zone are orthogonal in nature. If we assume the ARPES peak is a coherent object (as suggested by its relation with the superfluid
density), we must conclude that all other excitations in Brillouin Zone are incoherent, that is, their Fermi liquid spectral weight $Z$ should be zero. Especially, the nodal excitation should be incoherent. This may already be confirmed by ARPES experiment in both normal and superconducting state.\[11]\]

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[1] S.H. Pan et al, Nature (London) 403, 746 (2000).
[2] P.A. Lee, Phys. Rev. Lett. 71, 1887 (1993).
[3] J.M. Byers et al, Phys. Rev. Lett. 71, 3363 (1993).
[4] M.I. Salkola et al, Phys. Rev. Lett. 77, 1841 (1996).
[5] A. Polkovnikov et al, Phys. Rev. Lett. 86, 296 (2001).
[6] G. M. Zhang et al, Phys. Rev. Lett. 86, 704 (2001).
[7] J. X. Zhu et al, Phys. Rev. B 64, 060501 (2001).
[8] W. Rantner et al, Phys. Rev. Lett. 85, 3692-3695 (2000).
[9] A. Damascelli et al, Rev. Mod. Phys. 75, 473-541 (2003).
[10] F. Wilczek, cond-mat/0206122.
[11] T. A. Valla et al, Science 285, 2110 (1999).
FIGURES

FIG. 1. Momentum region of the ARPES peak in the Brillouin zone.

FIG. 2. Local density of state at the nearest-neighbouring site of Zinc contributed by the resonance. The thin line shows the contribution from ARPES peak in pure system.

FIG. 3. Real space distribution of the resonance. (a)Before $BiO$ layer filtering. (b)After $BiO$ layer filtering.
Differential Conductance

\[ \frac{\Delta I}{\Delta V} \]
