Impurity induced resonant state in a pseudogap state of a high temperature superconductor.

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We predict a resonance impurity state generated by the substitution of one Cu atom with a nonmagnetic atom, such as Zn, in the pseudogap state of a high-$T_c$ superconductor. The precise microscopic origin of the pseudogap is not important for this state to be formed, in particular this resonance will be present even in the absence of superconducting fluctuations in the normal state. In the presence of superconducting fluctuations, we predict the existence of a counterpart impurity peak on a symmetric bias. The nature of impurity resonance is similar to the previously studied resonance in the d-wave superconducting state.

The effects of a single magnetic and nonmagnetic impurity in high temperature superconductors have been studied intensively both theoretically \cite{1,2} and more recently experimentally by scanning tunneling microscopy (STM). Understanding of the impurity states in high-$T_c$ materials is important because impurity atoms qualitatively modify the superconducting properties, and these impurity induced changes can be used to identify the nature of the pairing state in superconductors.

Up to date theoretical analysis of the impurity states has been focused on the low temperature regime $T \ll T_c$, well below the superconducting transition temperature $T_c$. On the other hand it is well known that in the normal state ($T > T_c$) of underdoped cuprates, the electronic states at the Fermi energy are depleted due to pseudogap (PG) $\Delta_{PG}$, as was seen by STM \cite{3} and by angular resolved photoemission \cite{10}. One can consider the temperature evolution of the impurity state as the temperature increases and eventually becomes larger than $T_c$. There are two possibilities for the evolution of impurity resonance at $T > T_c$: a) the impurity resonance gradually broadens until the superconducting gap vanishes at which point the impurity resonance totally disappears and b) the resonance gets broader however survives above $T_c$. Which of the possibilities is realized depends on the normal state phase into which the superconductor evolves. It has been argued \cite{3,4} that in the underdoped regime the superconducting gap opens up in addition to the pseudogap present well above $T_c$. We find that the impurity resonance survives above $T_c$ in the pseudogap state of high-$T_c$ materials. The position and the width of the resonance are determined by the impurity scattering strength and PG scale. In the absence of a PG above $T_c$ the impurity state disappears.

The origin of PG state is one of the most strongly debated issues. Some models attribute PG to superconducting phase fluctuations above $T_c$ \cite{3}; others to a competing non-superconducting order parameter \cite{4}. Another possibility is that even within the PG regime there are at least two distinct sub-regimes – strong and weak pseudogaps, with weak pseudogap occurring at higher temperatures due to antiferromagnetic fluctuations, and strong pseudogap being related to superconducting fluctuations \cite{5,6}.

In this article we address the impurity induced resonance or quasibound state that is generated by a strong nonmagnetic impurity scattering in a CuO plane in the normal state of high-$T_c$ materials. Specifically we calculate the resonant state generated by the substitution of one Cu atom with a Zn atom using the self consistent $T$ matrix approach. We rely on the fact that the density of states (DOS) is depleted at the Fermi energy in the PG regime. We argue that the mere fact that DOS is depleted at the Fermi energy is sufficient to produce impurity resonance near the nonmagnetic impurity, such as Zn. However no particular use of the superconducting correlations above $T_c$ has been made in our analysis. For example, the results we present, will be valid in the PG state with no superconducting phase or amplitude fluctuations above $T_c$, as long as there are interactions that lead to the PG state, as indicated by a depleted DOS. This is an important caveat that broadens the validity of the model regardless of the microscopic origin of the PG in the high-$T_c$ superconductor. The approach we take is similar to the previous analysis of the nonmagnetic impurity in the superconducting state \cite{1}. See also figure 4.

The superconducting fluctuations are not required for the formation of the impurity state in the PG regime. However, in the presence of superconducting fluctuations an additional important feature of the impurity state is expected to appear. The natural quasiparticles in the superconducting state are the Bogoliubov quasiparticles, which are a linear combination of a particle and a hole. As a consequence, an impurity state in a superconductor appears both on positive (particle) and negative (hole) biases \cite{4,7}. In the phase-fluctuating pseudogap the Bogoliubov quasiparticles acquire a finite lifetime. However,
the particle-hole symmetry of the impurity states should remain to the extent to which the superconducting quasi-particles are defined [2]. Hence, the PG impurity states can serve as an extremely local probe able to distinguish between the superconducting and non-superconducting scenarios for the PG regime.

![Diagram of DOS in the pseudogap regime](image)

FIG. 1. An impurity state in a high Tc superconductor: (a) The DOS in the pseudogap regime used in this article (see also [11]) and (b) the DOS in the superconducting state as was used in [1]. In both phases there is a resonant state.

To be specific we need a model DOS that captures the main features of the PG in high-Tc materials. For this purpose we use the DOS that was measured [11] by Loram et al. In this work it has been argued that the DOS is a linearly vanishing function of energy within the ΔPG energy range near the Fermi surface, see figure 1(a).

We find that such a model indeed gives rise to an impurity bound state with energy Ω′ and decay rate Ω′′ equal to

\[ Ω = Ω' + iΩ'' = -\frac{Δ_{PG}}{2U N_0 \ln |2U N_0|} \left[ 1 + \frac{i\pi \text{ sign}(U)}{2 \ln |2U N_0|} \right], \tag{1} \]

where we have assumed the impurity scattering to be strong enough so that the result can be calculated to logarithmic accuracy with \[ \ln |2U N_0| > 1 \]. This is the main result of our work, which we will derive in the remainder of this paper.

The Hamiltonian for this single impurity problem is given by

\[ H_{\text{int}} = U n_0 = U \sum_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma}, \tag{2} \]

where U is the strength of the scalar impurity potential taken to be nonzero only at \( r = 0 \). The scattering matrix \[ G \] can be written as

\[ T = \frac{U}{1 - U \sum_k G_k(\omega)} = \frac{U}{1 - U G_0(\omega)}, \tag{3} \]

with \( G_0(\omega) \) the on site Green’s function \[ \text{[19]} \]. The states generated by the impurity are given by the poles of the T matrix:

\[ G_0(\Omega) = \frac{1}{U}. \tag{4} \]

This is an implicit equation for \( \Omega \) as a function of \( U \), the strength of the scattering. This solution can be complex, indicating the resonant nature of the virtual state. To solve this equation, we split \( G_0 \) into its imaginary and real part \( G_0 = G_0' + iG_0'' \). But also \( G_0''(\omega) = -\pi N_0(\omega) \) with \( N_0(\omega) \) the density of states.

Measurements on the electronic specific heat by Loram et al. [11] show that the normal state pseudo gap opens abruptly in the underdoped region below a hole doping equal to \( p_{\text{crit}} \sim 0.19 \) holes/CuO\(_2\). Inspired by these data, we will assume that around the pseudogap region, states are partly depleted and the density of states is linear, that is \( N(\omega) = N_0|\omega|/Δ_{PG} \) for \( |\omega| \leq Δ_{PG} \) and \( N(\omega) = N_0 \) for \( Δ_{PG} < |\omega| < W/2 \) with \( W \) the bandwidth. This density of states is depicted in figure 2(a). As it is obvious from the solution of equation (1), the precise position and the width of the resonance will depend on the specific form of the PG. We will use this linearly vanishing PG DOS. Results for the other form of \( N(\omega) \) can be obtained in a similar fashion [20].

From the Kramer–Kronig relation [2]

\[ G_0(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega' G_0'(\omega') P \left( \frac{1}{\omega' - \omega} \right), \tag{5} \]

with \( P \) Cauchy’s principle value, one can calculate the real part \( G_0' \) giving

\[ G_0'(\omega) = -N_0 \ln \left| \frac{\omega + \omega_0}{\omega - \omega_0} \right| + N_0 \ln \left| \frac{\Delta_{PG} - \omega}{\Delta_{PG} + \omega} \right| - N_0 \omega^2 \frac{\Delta_{PG}^2 - \omega^2}{\omega^2} \tag{6} \]

This function is depicted in figure 2(b) together with 1/\( U \). If 2\( U N_0 > e \), with \( e \) Euler’s constant, one can see from this figure that equation (6) has four solutions. But because the width of a resonance state is proportional to \( |\Omega| \), the only state with sharp width is the solution with \( |\Omega| \) close to zero and we will only consider this solution. After expansion in \( \omega \) of equation (6) we arrive at an expression for this solution \( \Omega \) of equation (1):

\[ G_0(\Omega) = -\frac{2\Omega N_0}{\Delta_{PG}} \left[ \ln \left| \frac{\Delta_{PG}}{\Omega} \right| - \frac{i\pi \text{ sign}(U)}{2} \right] = \frac{1}{U}, \tag{7} \]

which is solved to logarithmic accuracy by expression (6). Using this formula, taking \( N_0 = 1 \) state/eV, \( \Delta_{PG} \sim 300 K \sim 30 m eV \) and the scattering potential \( U \approx 4 e V \), we estimate \( \Omega \approx 20 K \sim 2 m e V \) as was found by Loram et al. [11]. This energy is close to the \( Z n \) resonance energy \( \omega_0 = 16 K \), seen in the superconducting state [21].

\[ \text{[19]} \]
The solution of the impurity state deep in the superconducting regime involves two aspects: the energy position and the width of the resonance and secondly, the real space shape of the impurity state. We have discussed the energy of the impurity state above. Great advantage of the on-site impurity solution is that only on-site propagator \( G_0(\omega) \) enters into calculation. Hence the knowledge of the DOS was sufficient to calculate the impurity state. On the other hand, to calculate the real space image of impurity induced resonance, one would require more detailed knowledge of the Green’s functions in the PG regime. Quite generally, one would expect for a d-wave like PG with nearly nodal points along the \((\pm \pi/2, \pm \pi/2)\) directions, that the impurity resonance in the pseudogap regime would be four-fold symmetric, similar to superconducting solutions of the solution of the equation \( G \).

FIG. 2. (a) The density of states \( N(\omega) = -G_0''(\omega)/\pi \). Around the pseudogap states are only partly depleted e.g. \( N(\omega) = N_0|\omega|/\Delta_{PG} \), where \( N(\omega) = N_0 \) for \( \Delta_{PG} < |\omega| < W/2 \) with \( W \) the bandwidth. (b) The real part \( G_0'(\omega) \) of Green’s function together with \( 1/U \) and \( U \) positive. \( \Omega' \) is the real part of the solution of the equation \( G_0'(\Omega) = 1/U \) to zero and therefore with sharp bandwidth. (c) The impurity induced resonance at \( \Omega' = -\Delta_{PG}/2U N_0 \ln(2U N_0) \). Because the other three solutions of equation (4) have much broader bandwidth, they are not depicted here. All the figures are taken on the impurity site.

This calculation would require a specific model for the PG state and goes beyond the scope of this paper.

While no superconductivity is required to form the impurity state in the PG, if the superconducting fluctuations are present then an additional satellite peak should appear on a symmetric bias due to the particle-hole nature of the Bogoliubov quasiparticles. The relative magnitude of the particle and the hole parts of the impurity spectrum can be used to determine the extent to which the PG is governed by the superconducting fluctuations. In the case of fully non-superconducting PG there should be no observable counterpart state. An optimal impurity for such determination would appear to be \( Nt \), which breaks the particle-hole symmetry more weakly than \( Zn \) even in the superconducting state. Combined with other experimental proposals [22,23], the impurity state can help to better understand the mysterious PG state.

In conclusion, we find the resonance state that is induced by the nonmagnetic impurity in the normal state of a high-\( T_c \) superconductor in the PG regime where the DOS at the Fermi surface is depleted. For the particular model of linear DOS we find that impurity state energy is given by equation (1). Impurity states survive at high temperature \( T > T_c \) since the PG produces the DOS depletion. This depletion is all that is necessary to produce the intragap state. In our solution we did not rely on a superconducting phase fluctuations above \( T_c \) to generate the impurity state. We estimated the energy of the \( Zn \) impurity resonance to be at \( 20K \), assuming a impurity potential equal to \( U = 4eV \). This resonance energy is indeed close to the energy of the \( Zn \) resonance at \( 16K \) in superconducting state [1].

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[18] The simplest model for thermal broadening is to assign the temperature dependent width: Thermal broadening at high temperatures $T > T_c$ substantially broaden the impurity resonance peak $\Omega''(T) = \sqrt{(\Omega''(T = 0))^2 + T^2}$.
[19] Even if there are any superconducting correlations in the d-wave pairing channel with an anomalous fluctuating propagator $F_k(\omega)$, it will not enter into the above equation. This is because regardless of the nature of the fluctuation we take $\sum_k F_k(\omega) = 0$ because of the d-wave ($\sim \cos(2\theta)$, where $\theta$ is the planar angle along the Fermi surface) nature of the pairing correlations.
[20] We argue that the appearance of the intragap impurity state is a robust feature of any depleted DOS around the Fermi surface. We also considered the model DOS with $N(\omega) = N_0 \left[ a + (1-a)\omega^2/\Delta_{PG}^2 \right]$ which leads essentially to similar results as a function of the impurity strength with a resonant state at $\Omega = -\Delta_{PG}(1 + i\pi a N_0 U)/(4N_0 U(1-a - \Delta_{PG}/W)) \approx -\Delta_{PG}(1 + i\pi a N_0 U)/(4N_0 U(1-a))$ when $\Delta_{PG}/W$ is small.
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