Impurity-induced resonant state in a pseudogap state of a high-T_c 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 this impurity resonance is similar to the previously studied resonance in the *d*-wave superconducting state.

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The effects of a single magnetic and nonmagnetic impurity in high-temperature superconductors have been studied intensively both theoretically[1–5] and, more recently, experimentally by scanning-tunneling microscopy (STM).[6–8] 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 now, 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 ($T \geqslant T_c$) of underdoped cuprates, the electronic states at the Fermi energy are depleted due to pseudogap (PG) Δ_{PG}, as was seen by STM[9] and by angular-resolved photoemission.[10] One can consider the temperature evolution of the impurity state as the temperature increases and eventually becomes larger than T_c. Then 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, the superconductor evolves into. It has been argued[11,12] that in the underdoped regime the superconducting gap opens up in addition to the pseudogap present well above T_c. Hence, 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 PG above T_c the impurity-state disappears.

The origin of the PG state is one of the most strongly debated issues. Some models attribute the PG to superconducting-phase fluctuations above T_c;[13] others to a competing nonsuperconducting order parameter.[14] Another possibility is that even within the PG regime there are at least two distinct subregimes—*strong* and *weak* pseudogaps, with a weak pseudogap occurring at higher temperatures due to antiferromagnetic fluctuations, and a strong pseudogap being related to superconducting fluctuations.[15,16]

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, the mere fact that the DOS is depleted at the Fermi energy is sufficient to produce a resonance near the nonmagnetic impurity, such as Zn. However *no particular use of the superconducting correlations above T_c is needed* 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.[1] See also Fig. 1.

The superconducting fluctuations are not required for the formation of the impurity state in the PG regime. However,

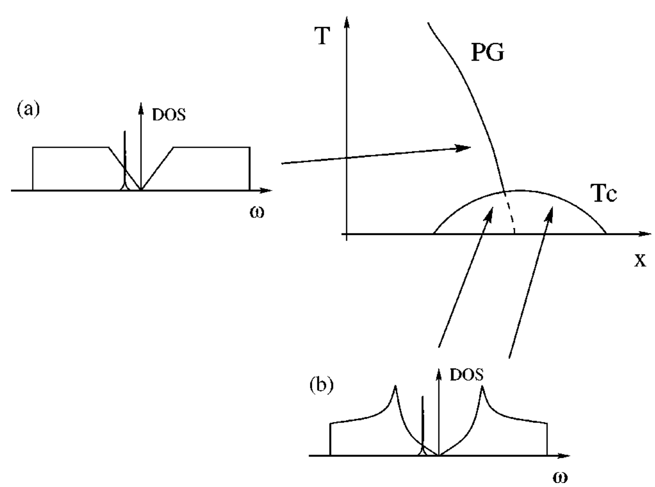

FIG. 1. An impurity state in a high T_c superconductor: (a) The DOS in the pseudogap regime used in this article (see also Ref. 11) and (b) the DOS in the superconducting state as was used in Ref. 1. In both phases there is a resonant state.

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. The Bogoliubov quasiparticles are linear combinations of electrons and holes, and hence their resonant bound states appear symmetrically both on positive (electron) and negative (hole) biases.[1,17] On the other hand, the electronic bound states are expected to appear on one bias only. This difference can be used to distinguish between the ''superconducting'' and the ''normal'' pseudogaps. If the PG state is related to the superconducting state, the Bogoliubov quasiparticles should still be present, although with a suppressed coherence length and short lifetime.[2] Atomic impurity is the ultimate microscopic probe, with the time resolution given by the inverse-resonant level width. Therefore, using different impurities with varying positions and widths of the resonant levels, one can determine the local temporal dynamics of the superconducting fluctuations above T_c, or possibly rule out the superconducting origin of pseudogap.

To be specific, we need a model DOS that captures the main features of the PG in high-T_c materials. For this purpose we use the DOS that was measured by Loram *et al.*[11] In this work, it has been shown that the DOS in the underdoped cuprates is a linearly vanishing function of energy within the interval $\Delta_{\rm PG}$ near the Fermi surface [see Fig. 1(a)]. We find that such DOS indeed gives rise to an impurity-bound state with energy Ω' and decay rate Ω'',

$$\Omega=\Omega'+i\Omega'' = -\frac{\Delta_{\rm PG}}{2UN_0}\frac{1}{\ln|2UN_0|}\left[1-\frac{1}{\ln|2UN_0|}+\frac{i\pi\ \ \mathrm{sgn}(U)}{2\ln|2UN_0|}\right], \tag{1}$$

where we have assumed the impurity scattering to be strong enough so that the result can be calculated to logarithmic accuracy with $\ln|2UN_0|>1$.[18] This is the main result, which we will derive in the remainder of this paper.

The Hamiltonian for the problem of single potential impurity of local strength U is given by

$$H=H_0+H_{\rm imp}, \tag{2}$$

$$H_{\rm imp}=U\hat{n}_0=U\sum_{\mathbf{k}\mathbf{k}'\sigma} c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}, \tag{3}$$

where H_0 is the Hamiltonian for the clean system, with the corresponding Green function $G_{\mathbf{k}}$. The scattering T matrix[1] can be written as

$$T=\frac{U}{1-U\sum_{\mathbf{k}} G_{\mathbf{k}}(\omega)}=\frac{U}{1-UG_0(\omega)}, \tag{4}$$

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

$$G_0(\Omega)=\frac{1}{U}. \tag{5}$$

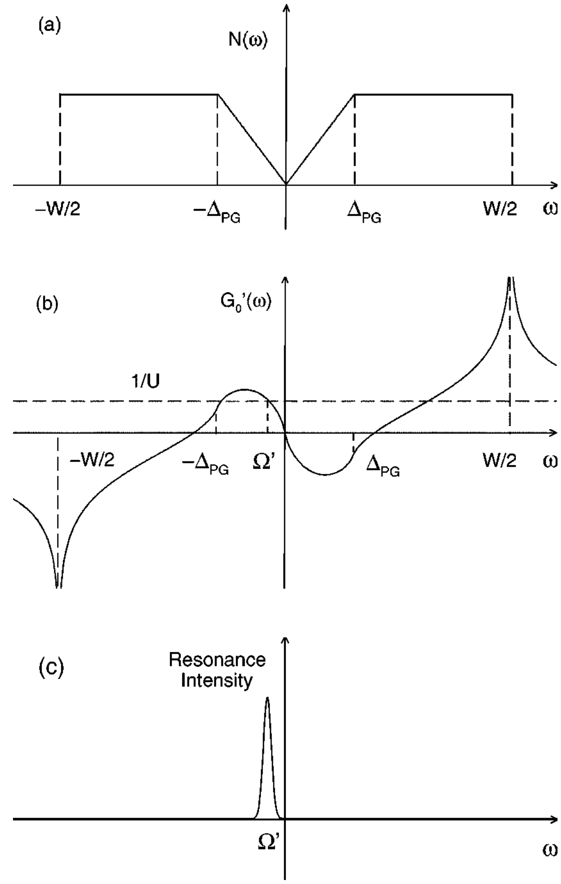

FIG. 2. (a) The density of states $N(\omega)=-G_0''(\omega)/\pi$. Around the pseudogap states are only partly depleted, e.g., $N(\omega)=N_0|\omega|/\Delta_{\rm PG}$, and $N(\omega)=N_0$ for $\Delta_{\rm PG}<|\omega|<W/2$ with W the bandwidth. (b) The real part $G_0'(\omega)$ of Green's function together with $1/U$ (U positive). Ω' is the real part of the solution of the equation $G_0(\Omega)=1/U$ close to zero and therefore with sharp bandwidth. (c) The impurity induced resonance at $\Omega'=-\Delta_{\rm PG}/2UN_0\ln(2UN_0)$. Because the other three solutions of Eq. (5) have much broader bandwidth, they are not depicted here. All the figures are taken on the impurity site.

This is an implicit equation for Ω 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 pseudogap opens abruptly in the underdoped region below a hole doping equal to $p_{crit}\sim 0.19$ 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 $N(\omega)=N_0|\omega|/\Delta_{\rm PG}$ for $|\omega|\leqslant\Delta_{\rm PG}$ and $N(\omega)=N_0$ for $\Delta_{\rm PG}<|\omega|<W/2$ with W the bandwidth. This density of states is depicted in Fig. 2(a). As it is obvious from the solution of Eq. (5), 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 other forms of $N(\omega)$

like a fully gapped DOS or a DOS with a quadratic dependent gap, can be obtained in a the same way and lead essentially to similar expressions.[20]

From the Kramer-Kronig relation[23]

$$G_0'(\omega)=\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega' G_0''(\omega')P\left(\frac{1}{\omega'-\omega}\right), \tag{6}$$

with P Cauchy's principle value, one can calculate the real-part G_0' giving

$$G_0'(\omega)=-N_0\ln\left|\frac{\frac{W}{2}-\omega}{\frac{W}{2}+\omega}\right|+N_0\ln\left|\frac{\Delta_{\rm PG}-\omega}{\Delta_{\rm PG}+\omega}\right| -N_0\frac{\omega}{\Delta_{\rm PG}}\ln\left|\frac{\Delta_{\rm PG}^2-\omega^2}{\omega^2}\right|. \tag{7}$$

This function is plotted in Fig. 2(b) together with $1/U$. If $2UN_0>1$, one can see from this figure that Eq. (5) 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 ω of Eq. (7) we arrive at an expression for this solution Ω of Eq (5):

$$G_0(\Omega)=-\frac{2\Omega N_0}{\Delta_{PG}}\left[\ln\left|\frac{\Delta_{PG}}{\Omega}\right|+1-\frac{i\pi\ \ \mathrm{sign}(U)}{2}\right]=\frac{1}{U}. \tag{8}$$

This equation can be solved exactly in terms of LambertW functions,[21] and to logarithmic accuracy it equals expression of Eq. (1).

Using formula (1), and taking $N_0=1$ state/eV, $\Delta_{\rm PG}\sim 300$ K~ 30 meV and the scattering potential $U\approx\pm 2$ eV, we estimate $\Omega\sim\pm 2$ meV$\sim\pm 20$ K as was found by Loram *et al.*[11] This energy is close to the Zn resonance energy $\omega_0=-16$ K, seen in the superconducting state.[6] By combining these results with the band-structure arguments,[22] we come to conclusion that the Zn impurity in Bi2212 is strongly attractive, with $U\sim -2$ eV. This result, as we will now see, may be modified due to the particle-hole asymmetry characteristic of doped cuprates.

In the absence of particle-hole symmetry, a similar calculation can be done. The simplest way to introduce the asymmetry is by making the upper and lower cutoffs in the DOS unequal. This situation corresponds to a chemical potential μ, located away from the center of the band. Keeping the DOS otherwise unchanged, with the pseudogap centered at the chemical potential, results only in the following change in the first logarithmic term of Eq. (7):

$$-N_0\ln\left|\frac{\frac{W}{2}-\mu-\omega}{\frac{W}{2}+\mu+\omega}\right|. \tag{9}$$

Neglecting the frequency ω relative to chemical potential μ and assuming that μ is small relative to the bandwidth, we obtain that the results for the asymmetric case can be obtained from the symmetric ones by the substitution

$$\frac{1}{U}\rightarrow\frac{1}{U}-\frac{4N_0\mu}{W}. \tag{10}$$

The effect of the asymmetry term can be estimated for superconducting cuprates. For 20% hole doping, $\mu\sim-(1/5)W/2=-W/10$. Hence, the modified value for the Zn impurity strength in Bi2212 can be obtained from the symmetric result, $1/U^*=1/U+4N_0\mu/W$. The new value is $U^*\sim -1$ eV, which is a strongly attractive potential, as is expected from the band-structure arguments.

The solution of the impurity state deep in the superconducting regime involves two aspects: first, the energy position and the width of the resonance and second, 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 for the localized potential U 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-wavelike 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.[1–8] 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 nonsuperconducting PG there should be no observable counterpart state. An optimal impurity for such determination would appear to be Ni, which unlike Zn, doesn't significantly suppress superconductivity in its vicinity. Combined with other experimental proposals,[24,25] 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. For the particular model of linearly vanishing DOS we find the impurity-state energy, Eq. (1). We also analyze the effects of the particle-hole asymmetry. 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. While the existence of the resonance state does not rely on superconducting-phase fluctuations above T_c, in the presence of such fluctuations *two* peaks are expected to appear on symmetric biases. We propose this effect as an experimental method that can distinguish between the superconducting and nonsuperconducting origin of pseudogap.

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[17] A. Yazdani, B.A. Jones, C.P. Lutz, M.F. Crommie, and D.M. Eigler, Science **275**, 1767 (1997).

[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 $F_{\mathbf{k}}(\omega)$, it will not enter into the above equation. This is because regardless of the nature of the fluctuation we take $\Sigma_{\mathbf{k}} F_{\mathbf{k}}(\omega) = 0$ because of the *d*-wave $[\sim \cos(2\theta)$, where θ 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 $N(\omega) = N_0[a + (1-a)\omega^2/\Delta_{PG}^2]$ that 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 Δ_{PG}/W is small. But also a fully gapped DOS equal to $N(\omega) = N_0$ for $|\omega| \in [\Delta_{PG}, W/2]$ and zero otherwise gives rise to a comparable expression with a resonant state at $\Omega = -\Delta_{PG}/(2UN_0)$.

[21] The exact solution in terms of a LambertW function, $Lw(-1,x)$, is $\Omega = -\Delta_{PG}\mathrm{sign}[U]\exp(Lw(-1, -\mathrm{sign}[U]\exp[i\pi/2-1]/(2N_0U)) + 1 - i\pi/2)$, where $Lw(x)$ is such that $Lw(x)\exp Lw(x) = x$.

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