Resonant Impurity States in the D-Density-Wave Phase

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We study the electronic structure near impurities in the d-density-wave (DDW) state, a possible candidate phase for the pseudo-gap region of the high-temperature superconductors. We show that the local DOS near a non-magnetic impurity in the DDW state is qualitatively different from that in a superconductor with $d_{x^2−y^2}$-symmetry. Since this result is a robust feature of the DDW phase, it can help to identify the nature of the two different phases recently observed by scanning tunneling microscopy experiments in the superconducting state of underdoped Bi-2212 compounds.

71.55.-i, 72.10.Fk, 71.10.Hf, 74.72.-h

The pseudogap region of the high-temperature superconductors (HTSC) has attracted considerable theoretical and experimental attention over the last few years. Recent scanning tunneling microscopy (STM) experiments in the superconducting state of underdoped Bi-2212 compounds have observed regions with two qualitatively different density of states (DOS). These regions are referred to as the α and β phases. While the DOS in the α phase resembles that of a superconductor with $d_{x^2−y^2}$-symmetry, the DOS in the β phase is similar to that observed in the pseudogap phase of the underdoped HTSC. A series of papers have proposed that the pseudo-gap region arises from the presence of a d-density-wave (DDW) phase; a current-carrying state with $d_{x^2−y^2}$-symmetry. Whether the β phase can be identified with the DDW state is currently a topic of intense discussion.

In this Letter we suggest that the nature of the observed phases can be clarified by considering the electronic structure in the vicinity of impurities. We show, using a $T$-matrix approach, that the local DOS near a non-magnetic impurity in the DDW state is qualitatively different from that in a superconductor with $d_{x^2−y^2}$-symmetry (DSC). While the DDW-DOS near an impurity changes with the specific form of the normal state band structure, its qualitative differences to the DOS in a DSC remain. They are therefore robust features of the DDW phase which can they shed important insight into and discriminate between the α and β phases observed in Refs. Finally, we show that a magnetic impurity induces two resonance states in the DDW-DOS, a result which is qualitatively similar to that in a DSC.

Starting point for our calculations is the $T$-matrix formalism for a single impurity in the DDW state. We introduce the spinor

$$\Psi_{k,\alpha} = \left(c_{k,\alpha}^\dagger, c_{k+Q,\alpha}^\dagger\right), \quad (1)$$

where $\alpha$ is the spin index, such that the electronic Greens function is given by $G_{\alpha,\alpha}(k, \tau - \tau') = -\langle T \Psi_{k,\alpha}(\tau) \Psi_{k,\alpha}(\tau') \rangle$. In what follows we omit the spin index, since for the cases considered below $\tilde{G}$ is independent of $\alpha$. In the clean limit one has

$$\tilde{G}^{-1}_{0}\left(k, \omega_n\right) = \begin{pmatrix} i\omega - \epsilon_k & i\Delta_k \\ -i\Delta_k & i\omega - \epsilon_{k+Q} \end{pmatrix}, \quad (2)$$

where $\Delta_k = \Delta_0(\cos k_x - \cos k_y)/2$ is the DDW gap, $Q = (\pi, \pi)$ is the ordering moment of the DDW state. The normal state electronic dispersion is given by

$$\epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu, \quad (3)$$

where $t, t'$ are the hopping elements between nearest and next-nearest neighbors, respectively, and $\mu$ is the chemical potential. In the following we use $t = 300$ meV, $\Delta_0 = 50$ meV, and values for $t'$ and $\mu$ as discussed below.

We first consider a non-magnetic impurity described by the scattering Hamiltonian

$$\mathcal{H}_{sc} = U_0 \sum_{k,k',\alpha} \hat{\Psi}_{k,\alpha}^\dagger \hat{T} \hat{\Psi}_{k',\alpha}, \quad (4)$$

where $U_0$ is the scattering strength of the impurity, the prime restricts the summation to the momenta in the Brillouin zone (BZ) of the DDW state, $\hat{T} = 1 + \hat{r}_2, \hat{r}_1$ is the unit matrix and $\hat{r}_a$ are the Pauli matrices in spinor space. In the presence of this scattering potential the Greens function is given by

$$\tilde{G}(r, r', \omega_n) = \tilde{G}_0(r' - r, \omega_n) + \tilde{G}_0(-r, \omega_n) \hat{T}(\omega_n) \tilde{G}_0(r', \omega_n), \quad (5)$$

where one has for the $T$-matrix

$$\hat{T}(\omega_n) = \left[1 - U_0 \hat{T} \tilde{G}_0(0, \omega_n)\right]^{-1} U_0 \hat{T}. \quad (6)$$

For the change in the electron Greens function due to the impurity scattering one obtains

$$\delta \tilde{G}_{11}(r, \omega_n) = U_0 \left[\tilde{G}_{11}(0, \omega_n)\right]^2 - \frac{\left[\tilde{G}_{11}(r, \omega_n)\right]^2}{1 - U_0 \tilde{G}_{11}(0, \omega_n)}, \quad (7)$$

Note, that for a given scattering strength, $U_0$, there exist only a single resonant state at a frequency, $\omega_{res}$, where the real part of the denominator on the r.h.s. of Eq. (7)
vanishes. We first consider an electronic structure in the normal state, Eq. (3), with \( t' = 0 \) and at half-filling, \( \mu = 0 \). We present our numerical results for the DDW-DOS

\[
N(\omega) = -\frac{2}{\pi} \text{Im} \tilde{G}^{(11)}(r, r, \omega + i\delta),
\]

in the absence of an impurity (clean case) and for a single non-magnetic impurity with scattering strength \( U_0 = 1 \text{ eV} \) in Fig. 1. The DDW-DOS in the clean case (solid line) vanishes linearly at small frequencies, and exhibits two peaks at \( \pm \Delta_0 \). As discussed above, a single resonance state appears at the impurity site (dashed line). For \( U_0 > 0 ( < 0 ) \), this resonant state is located at \( \omega_{r,\Delta} = 0 \), i.e., on the particle (hole) site. In the DOS on the impurity’s nearest-neighbor site (dotted line) the resonant state remains particle-like with an amplitude which is larger than that on the impurity site itself. This is to be expected since at the impurity site, \( \tilde{G}_0^{(11)}(0, \omega_{r,\Delta}) \neq 0 \). In the limit \( U_0 \to \infty \), the spectral weight of the resonance at the impurity site, \( U_0[\tilde{G}_0^{(11)}(0, \omega_{r,\Delta})]^2 \) vanishes. The DOS on the impurity’s next-nearest-neighbor site exhibits barely any resonant enhancement, while the peaks at the gap edges are still suppressed. Thus, as one moves away from the impurity site, the signature of the resonance states in the DOS are lost before the gap edge peaks are recovered.

We now compare the above results for the DOS with those near a non-magnetic impurity in a superconductor with \( d_{x^2-y^2} \)-symmetry. Here, the correction to the Greens function arising from the impurity scattering is given by

\[
\delta G(r, i\omega_n) = \frac{U_0 [G_0(r, i\omega_n)]^2}{1 - U_0 G_0(0, i\omega_n)} - \frac{U_0 [F_0(r, i\omega_n)]^2}{1 - U_0 G_0(0, -i\omega_n)},
\]

where \( G_0, F_0 \) are the normal and anomalous Greens functions in the SC state, respectively. Due to the particle-hole mixing in the SC state, there exist in general two resonance states at frequencies where the denominators on the r.h.s. of Eq. (3) vanish. Note, that the spectral weight of these states is determined by \( [G_0(r, i\omega_n)]^2, [F_0(r, i\omega_n)]^2 \), respectively. In Fig. 2 we present the DOS near the impurity site for \( U_0 = 1 \text{ eV} \), and the same set of band parameters as in Fig. 1. The SC DOS in the clean limit (solid line) is identical to that in the DDW state (solid line in Fig. 1). The DOS at the impurity site exhibits a single resonance state, since the spectral weight of the second resonance vanishes, \( [F_0(0, i\omega_n)]^2 \equiv 0 \). For \( U_0 > 0 ( < 0 ) \), the resonance state is located at \( \omega_{r,\Delta} = 0 \) (\( > 0 \)), i.e., on the particle (hole) site. While this result is similar to that in the DDW state (dashed line in Fig. 1), the DOS on the impurity’s nearest-neighbor site is qualitatively different (dotted line). Since here the spectral weight of both resonances is non-zero, \( [G_0(r, i\omega_n)]^2, [F_0(r, i\omega_n)]^2 \neq 0 \), the DOS exhibits two resonance states. We find that in general, i.e., independent of the specific band structure, the hole-like resonance possesses the larger spectral weight, \( [F_0(r, i\omega_n)]^2 > [G_0(r, i\omega_n)]^2 \). Similar results were obtained earlier in Refs. [9]. Thus, the spatial dependence of the DOS near a non-magnetic impurity can be used to determine the broken-symmetry phase in which the impurity is embedded. A similar conclusion was recently reached by Zhu et al. [11]. Note, that the appearance of a resonance state at the impurity site only requires a suppression of the DOS at low frequencies [10], but not...
necessarily a broken symmetry phase.

We next consider the electronic states in the vicinity of a magnetic impurity described by the scattering Hamiltonian

$$\mathcal{H}_{sc} = -JS \sum_{\mathbf{k},\mathbf{k}',\alpha,\beta} \hat{T}_{\mathbf{k},\alpha} \hat{\sigma}_{\alpha,\beta} \Psi_{\mathbf{k}',\beta}$$

(10)

where $S = 1/2$ and $\hat{\sigma}$ are the Pauli-matrices in spin space. For the $\hat{T}$-matrix one has [11]

$$\hat{T}(i\omega_n) = \left[ 1 - \left( \beta \hat{T}_0(0, i\omega_n) \right)^2 \right]^{-1} \hat{T}_0(0, i\omega_n) \hat{T}_0$$

(11)

with $\beta = JS$. The correction to the Greens function arising from the impurity scattering is given by

$$\delta \hat{G}^{(11)}(\mathbf{r}, i\omega_n) = \frac{\beta^2 \hat{G}^{(11)}_0(0, \omega)}{1 - \beta^2 \left[ \hat{G}^{(11)}_0(0, \omega) \right]^2} \times \left\{ \hat{G}^{(11)}_0(\mathbf{r}, i\omega_n) \right\}^2 + \left[ \hat{G}^{(12)}_0(\mathbf{r}, i\omega_n) \right]^2$$

(12)

Note, that a magnetic impurity in the DDW state induces two resonance states with equal spectral weight. In Fig. 3 we present the DOS in the clean case and for a single magnetic impurity with scattering strength $\beta = 1$ eV. The resonance states again possess a larger spectral weight at the nearest-neighbor site than on the impurity site itself. Similar to the case of a non-magnetic impurity, the DOS on the next-nearest-neighbor site exhibits barely any resonant enhancement, while the peaks at the gap edges are still suppressed. These results are qualitatively similar to those obtained for a magnetic impurity in a dSC.

So far, we have only discussed the DOS near an impurity for the half-filled case and $t' = 0$. We next address the question of how robust the above results are against changes in the band structure. In particular, we consider a set of band parameters which describes the FS measured by ARPES experiments in Bi-2212 [12]. To this end we take $t' = -0.3t$ and $\mu = -0.91t$, which corresponds to a hole doping of 10\%, characteristic of the underdoped HTSC. The resulting Fermi surface in the DDW state is shown in Fig. 4a. In contrast to the case considered above with $t' = \mu = 0$, where the FS only consists of four Fermi points at $\mathbf{q} = (\pi/2, \pm \pi/2)$, the FS now exhibits hole pockets centered around $\mathbf{q}_c$. This form of the FS immediately implies that the DOS (in the clean case) at zero energy is now non-zero, in contrast to the results shown.

FIG. 3. DDW-DOS for the clean case (solid line) and in the presence of a magnetic impurity with $\beta = 1$ eV: (1) DOS on the impurity site, (2) DOS on the nearest-neighbor site, and (3) DOS on the next-nearest-neighbor site.

FIG. 4. (a) Fermi surface in the DDW state with $t' = -0.3t$, $\mu = -0.91t$ (corresponding to a hole doping of 10\%) and $\Delta_0 = 50$ meV. The hole pockets are centered around $(\pm \pi/2, \pm \pi/2)$. (b) DOS in the DDW state with the same band parameters as in (a), for the clean case (solid line) and in the presence of a non-magnetic impurity with $U_0 = 1$ eV: (1) DOS on the impurity site, (2) DOS on the nearest-neighbor site, and (3) DOS on the next-nearest-neighbor site. Inset: SC DOS for the same band parameters as in (a).
in Fig. 4b. This is confirmed by our numerical evaluation of the DOS which we present in Fig. 4b. In the clean case (solid line) the DOS exhibits two peaks at $\omega \approx -126$ and $-35$ meV, which correspond to the two peaks at $\omega = \pm 50$ meV for $t' = \mu = 0$ (see Fig. 1). Thus, the DOS for non-zero $t'$ and hole-doping is shifted downwards in energy, in comparison to the case $t' = \mu = 0$. Since the DOS in Fig. 4b does not show any significant reduction at low energies, we expect that any resonance state near an impurity couples strongly to the continuum of electronic states, which in turn reduces its amplitude and spectral weight. Our numerical results for the DOS near a non-magnetic impurity with $U_0 = 1$ eV as shown in Fig. 4b confirm this conclusion. While the DOS at the impurity site is again reduced in comparison to the clean case, it does not exhibit any signature of a resonance state. In contrast, the DOS in the SC state remains qualitatively unchanged from the case $t' = \mu = 0$, as shown in the inset of Fig. 4b. We obtain qualitatively similar results to those shown in Fig. 4b for a variety of doping concentrations and values of $t'$. We thus conclude that the DOS in the DDW phase remains qualitatively different from that in a dSC for a wide range of electronic band structures and chemical potentials. Our results are therefore robust features of the DDW phase and can discriminate it from other broken-symmetry phases.

The clean DOS in the DDW state for $t' = \mu = 0$ (Fig. 1) is in good qualitative agreement with the results presented in Refs. [2]. The DDW-DOS for $t' = -0.3t$ and 10% hole doping (Fig. 4b), however, does not show a reduction at low frequencies, and thus apparently disagrees with the experimental data. Here, we propose two explanations to resolve this apparent discrepancy. First, the differences between the $\alpha$ and $\beta$ phases could arise from doping inhomogeneities on the $20 - 30$ Å scale, with the $\alpha(\beta)$ phase containing the higher (lower) hole concentration. According to the phase diagram proposed in Ref. [1], the $\beta$ phase then corresponds to the DDW state, while the $\alpha$ phase is a dSC. In this case, the DDW-DOS is expected to be similar to that shown in Figs. 1 and 2 (small $\mu$ limit), while the dSC-DOS resembles our results in the inset of Fig. 4b (large $\mu$ limit), in qualitative agreement with the experimental data. Second, it was argued that the interaction with the spin susceptibility, $\chi$, peaked at $Q = (\pi, \pi)$, substantially changes the properties of electrons in those regions of the FS which can be connected by $Q$ (hot spots) [13,14]. In particular, it was shown that for the underdoped HTSC, this interaction leads to a suppression of the DOS at low frequencies and a shift of spectral weight to higher energies [13,14]. Since the FS in the DDW state (see Fig. 4b) exhibits a high degree of nesting with wave-vector $Q$, we expect that the interaction with spin excitations yields the same kind of suppression in the low frequency DDW-DOS. This suppression then leads to a reappearance of resonance states near the impurity site. Work to explore this possibility is currently under way [13]. If this conjecture turns out to be correct, the suppression of the low energy DDW-DOS would be a robust feature and independent of the particular form of the FS in the normal state.

In conclusion, we have shown that a non-magnetic impurity in the DDW state induces a resonance state in the local DOS. At half-filling and $t' = 0$ we argue that the spatial dependence of this resonance peak is qualitatively different from that in a superconductor with $d_{x^2-y^2}$-symmetry. Since away from half-filling, the qualitative differences between the DDW-DOS and the dSC-DOS remain, they are robust features of the DDW phase and can thus shed important insight into the nature of the $\alpha$ and $\beta$ phases observed in underdoped Bi-2212 [2]. Finally, we show that a magnetic impurity induces two resonance states in the DDW-DOS, a result which is qualitatively similar to that in a dSC.

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