Identifying Collective Modes via Impurities in the Cuprate Superconductors

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We show that the pinning of collective charge and spin modes by impurities in the cuprate superconductors leads to qualitatively different fingerprints in the local density of states (LDOS). In particular, we find that the coupling of impurities with spin and charge droplets gives rise to characteristic spatial patterns of the spin-resolved LDOS. Since all of these fingerprints are absent in a charge droplet, impurities are a new probe for identifying the nature and relative strength of collective modes.

Whether the unconventional properties of the high-temperature superconductors (HTSC) arise from the interaction of electronic degrees of freedom with collective spin modes, charge modes, or phonons, is one of the key issues in understanding these complex materials [1]. While some angle-resolved photoemission (ARPES) experiments [2] observed effects of the magnetic resonance mode [3, 4] on electronic excitations, other ARPES studies argued that the electronic dispersion exhibits a number of prominent features that arise from the coupling to phonons [5]. Moreover, recent scanning tunneling spectroscopy (STS) experiments [6] have reported evidence that are inconsistent with those of the magnetic resonance mode [4, 7]. The interpretation of these experiments is further complicated by the coupling between impurities and collective spin and charge modes and phonons [5].

In this Letter, we propose that STS experiments can directly address this issue by studying the effects in the LDOS of a $d_{x^2−y^2}$-wave superconductor that arise from a coupling between impurities and collective spin and charge modes. In particular, we show that such a coupling induces a static spin (charge) density droplet which represents an extended scattering potential for the electronic degrees of freedom and thereby affects the superconductor’s local electronic structure. Indeed, static spin droplets around Ni and Zn impurities have been observed in nuclear magnetic resonance (NMR) experiments [8, 10, 11, 12]. By using the $T$-matrix [13] and Bogoliubov-de Gennes (BdG) [13] formalisms, we demonstrate that scattering off spin and charge droplets gives rise to qualitatively different fingerprints in the superconductor’s LDOS. In particular, we find that the coupling of an impurity to a spin mode peaked at $Q = (\pi, \pi)$ prevents the creation of a resonant impurity state, leading to characteristic spatial patterns of the spin-resolved LDOS directly reflecting the mode’s antiferromagnetic nature, and gives rise to a pronounced magnetic field dependence of the LDOS. Since all of these features are absent in the presence of a charge droplet, our results demonstrate that impurities can be used to identify the nature and relative strength of collective modes not only in the HTSC, but in strongly correlated electron systems in general.

The coupling of a single impurity with spin $s_{\text{imp}}$ located at site $R$ to collective spin and charge modes, represented by the operators $s_c$ and $n_c$, respectively, is described by the Hamiltonian [16, 17]

$$H_{\text{int}} = -JS_{\text{imp}} \cdot s_c(R) + Un_{\text{imp}} n_c(R)$$

with $J, U > 0$ and $(n_{\text{imp}}) = 1$. Note that the creation of a static spin droplet requires a non-zero spin polarization of the impurity, $\langle S^z_{\text{imp}} \rangle$, which can be induced, for example, by applying a magnetic field $H \ll H_{ab}^m$ in the $ab$-plane thus avoiding complications arising from the creation of vortices [18]. Experimentally, $\langle S^z_{\text{imp}} \rangle = C/(T + \Theta)$ obeys the Curie-Weiss law [12]. The impurity-mode coupling of Eq. (1) induces static spin [16] and charge density oscillations [17] described by

$$\langle s^z_c(r) \rangle = J\langle S^z_{\text{imp}} \rangle \chi_s(r - R, \omega = 0),$$
$$\langle \delta n_c(r) \rangle = U\langle n_{\text{imp}} \rangle \chi_c(r - R, \omega = 0),$$

respectively. Here, $\chi_s(\omega)$ is the spin (charge) susceptibility, $\delta n_c(\omega) = n_c(\omega) - n_0$, and $n_0$ is the uniform charge density. For the static susceptibilities in momentum space, we make the ansatz $\chi_{s,c}(q, \omega = 0) = \chi_{s,c}^{\text{imp}}/(\xi_{s,c}^2 + (q - Q_{s,c})^2)$ where $\xi_{s,c}$ is the respective correlation length, $Q_s = (\pi, \pi)$ [20] and hence $Q_c = 0$, in agreement with NMR experiments [8, 10, 11, 12, 16, 21]. The mean-field Hamiltonian of the entire system is given by

$$H = \sum_{r,r',\sigma} t_{rr'} c_{r,\sigma}^\dagger c_{r',\sigma} + \sum_{r, \sigma} \left[ \Delta_{r, r'} c_{r, \sigma}^\dagger c_{r', \sigma}^\dagger + h.c. \right]$$
$$- \sum_{r, \alpha} \left[ g_s(s_z(r)) \sigma_{\alpha, \beta} - g_c(\delta n(r)) \ell_{\alpha, \beta} \right] c_{r, \alpha}^\dagger c_{r, \beta} ,$$

where $c_{r, \sigma}^\dagger$ creates an electron with spin $\sigma$ at site $r$, $t_{rr'}$ is the hopping integral between sites $r$ and $r'$, and $\Delta_{r, r'}$ is the $d_{x^2−y^2}$-wave superconducting (SC) gap. The last
term in Eq. (3) describes the scattering of electrons by the total spin density \( \langle s_z(r) \rangle = \langle \sigma_z^2 \rangle \) and effective charge density \( \langle \delta n(r) \rangle = \langle \delta n_c(r) \rangle + \delta n_{R,R} \langle \delta n_{imp} \rangle \). The droplets’ scattering strength is determined by only two parameters: for a spin droplet by \( \eta_s = J_\chi_s(0,0) \) and \( g_s = g_s(S_{imp}) \), such that \( g_s(s_z(r)) = g_s [\eta_s \chi_s(r - R, 0)/\chi_s(0,0) + \delta n_{R,R}] \), and for a charge droplet by \( \eta_c = U \chi_c(0,0) \) and \( g_c = g_c(n_{imp}) \).

We study the effects of electronic scattering on the LDOS by using two complementary methods: the \( T \)-matrix \([13, 14]\) approach, which allows us to investigate large host systems but assumes a spatially constant SC order parameter (SCOP), and the Bogoliubov-de Gennes (BdG) \([15]\) formalism, which accounts for spatial variations of the SCOP, but can only treat small system sizes. Within the \( T \)-matrix approach, the Green’s function matrix in Matsubara space is given by \([14]\)

\[
\hat{G}(r', r, \omega_n) = \hat{G}_0(r', r, \omega_n) + \sum_{l,p} \hat{G}_0(l, \omega_n) \hat{T}(l, p, \omega_n) \hat{G}_0(p, r', \omega_n), \tag{4}
\]

where the sum runs over all droplet sites. The \( \hat{T} \)-matrix is determined from

\[
\hat{T}(l, p, \omega_n) = \hat{V}_l \delta_{l_p} + \hat{V}_l \sum_s \hat{G}_0(l, s, \omega_n) \hat{T}(s, p, \omega_n), \tag{5}
\]

where \( \hat{G}_0 = [\omega_n \sigma_0 - \varepsilon_k \sigma^3 + \Delta_k \sigma_1]^{-1} \) is the unperturbed Green’s function, \( \hat{V}_l = -g_s(s_z(l)) \sigma^2 + g_c(\delta n(l)) I \), \( \varepsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu \) is the normal state tight binding dispersion with \( t = 300 \) meV, \( t'/t = -0.4 \), and \( \mu/t = -1.083 \), representative of the HTSC \([22]\), and \( \Delta_k = \Delta_0(\cos k_x - \cos k_y)/2 \) is the SC gap with \( \Delta_0 = 30 \) meV. The LDOS, \( N(r, \omega) = A_{11}(r, \omega) - A_{22}(r, \omega) \) with \( A_j(r, \omega) = -\text{Im} \hat{G}_{ii}(r, \omega + i\delta)/\pi \) and \( \delta = 0.2 \) meV is obtained from Eq. (4). In contrast, in the BdG formalism \([15]\), one solves the eigenvalue equation

\[
\sum_{r'} \left( \frac{H^+_{rr'} - H^-_{rr'}}{\Delta_{rr'}} \right) (u_{r,n}, v_{r',n}) = E_n (u_{r,n}, v_{r,n}) \tag{6}
\]

with \( H^\pm_{rr'} = t_{rr'} + (\mp g_s(s_z(r)) - g_c(n(r)) - \mu) \delta_{r,r'} \), and self-consistently computes the SC gap via

\[
\Delta_{rr'} = -\frac{1}{2} \sum_n [u_n(r) v_n(r') + u_n(r') v_n(r)] \tanh \left( \frac{E_n}{2k_B T} \right), \tag{7}
\]

where the sum runs over all eigenstates of the system, and \( V = 0.7375 \) \( t \) yields the same (clean) SC gap as taken in the \( T \)-matrix approach. The LDOS is obtained via

\[
N(\omega, r) = \sum_n \left[ u^2_n(r) \delta(\omega - E_n) + v^2_n(r) \delta(\omega + E_n) \right].
\]

In order to identify the qualitative effects of spin and charge droplets on the LDOS, we first consider the case when only one of the modes couples to the impurity and present in Fig. 1(a) [(b)] the normalized spin (charge) density for a pure spin (charge) droplet [the center of the droplet is located at \( (0,0) \)] \([23]\). To directly compare the effects of the droplets, we use \( g_s = g_c \) and \( \xi_s = \xi_c \) with \( \xi = 5\xi_0 \) representative of the underdoped HTSC \([11]\) and present in Figs. 1(c) and (d) the LDOS obtained from the \( T \)-matrix approach inside the spin and charge droplet, respectively. The low-frequency LDOS in these two droplets exhibits significant qualitative differences. Inside the spin droplet, the SC coherence peaks are clearly visible and no impurity resonance exists inside the SC gap (the LDOS exhibits, however, weak Friedel-like oscillations). In contrast, inside the charge droplet, the SC coherence peaks are strongly suppressed and a resonant impurity state is formed with peaks in the LDOS at \( \pm 2 \) meV. These qualitatively different effects of the charge and spin droplet on the LDOS arise from the spatial forms of their scattering potentials. For a spin droplet, the alternating sign of \( s_z(r) \) and hence of the scattering potential leads to destructive interference of scattered electrons which prevents the creation of an impurity state inside the SC gap. This interpretation is supported by the fact that the impurity resonance of the decoupled \( (\eta_s = 0) \) impurity [see Fig. 1(c)] shifts to higher energies with increasing \( \eta_s \), implying a decrease in the effective scattering strength of the im-

FIG. 1: (color online) Normalized spin (a) and charge (b) density along \( r = (x, 0) \). LDOS inside a spin (c) and charge (d) droplet with \( \eta_s = 1 \) and \( g_s, g_c = 400 \) meV (the dashed lines represent the clean LDOS). Evolution of the LDOS with increasing \( \eta_s,c \) for a spin (e) and charge (f) droplet.
purity. Note that for sufficiently large $\eta_s$, the LDOS is qualitatively different from that of a decoupled impurity ($\eta_c = 0$). In contrast, for the charge droplet, the scattered electrons interfere constructively due to the same sign of the scattering potential at all sites, which leads to an increase in the effective scattering strength. Accordingly, the impurity resonance of the decoupled ($\eta_c = 0$) impurity shifts to lower energies with increasing $\eta_c$ [see Fig. 1(f)]. The modes’ different momentum dependence thus leads to distinct fingerprints of a spin [Fig. 1(c)] and charge [Fig. 1(d)] droplet in the LDOS.

Another important fingerprint of the spin droplet can be found in the spatial structure of the spin-resolved LDOS, as shown in Fig. 2(a) and (b) where we present the spin↑ and spin↓ LDOS at adjacent sites. As expected from the spatially alternating sign of the scattering potential, the frequency dependence of the spin-resolved LDOS is large, the spin↓ LDOS at $\omega_{cp} = 30$ meV.

![Figure 2](image)

**FIG. 2:** (color online) Spin resolved LDOS for $\tilde{g}_s = 400$ meV at adjacent sites (a) $r = (1,0)$, and (b) $r = (2,0)$. Intensity plot of the (c) spin↑ and (d) spin↓ LDOS at $\omega_{cp} = 30$ meV. From the intensity pattern, as shown in Figs. 2(c) and (d) where we present an intensity plot of the spin-resolved LDOS at the frequency of the hole-like coherence peak, $\omega_{cp} = 30$ meV. At sites where the spin↑ LDOS is large, the spin↓ LDOS is small, and vice versa. In contrast, in a charge droplet, the spin↑ and spin↓ LDOS are identical. Hence, the qualitatively different behavior of the spin-resolved LDOS in spin and charge droplets is directly linked to the magnetic/non-magnetic nature of the modes.

Another qualitative difference between spin and charge droplets arises from the magnetic field dependence of the impurity’s spin polarization $\langle S_{imp}^z(H,T) \rangle = CH/(T+\Theta)$ [12]. Since $\tilde{g}_s = g_s \langle S_{imp}^z(H,T) \rangle$, it immediately follows that the droplet’s scattering strength and hence the resulting LDOS are expected to change with $H$ and $T$.

To demonstrate this effect, we present in Fig. 3(a) the total LDOS for several values of $\tilde{g}_s$ representing different magnetic fields. Consider, for example, that a given $H_0 \ll H_{ab}^0$ corresponds to $\tilde{g}_s = 100$ meV. Increasing the magnetic field to $2H_0$, ($\tilde{g}_s = 200$ meV) or $4H_0$ ($\tilde{g}_s = 400$ meV) leads to a suppression of the LDOS in the droplet [24]. Since the coupling between impurity and a charge mode is unaffected by the magnetic field, the observation of a magnetic field dependent LDOS as shown in Fig. 3(a) is another direct signature of a static spin droplet.

If both charge and a spin modes are present in the superconductor and simultaneously couple to an impurity, we find that properties of the resulting LDOS are predominantly determined by the ratio $\alpha = \tilde{g}_c \eta_c / (\tilde{g}_s \eta_s)$, as shown in Fig. 3(b) for $\alpha = 1/3$. As $\alpha$ changes from 0 to $\infty$, the LDOS changes continuously from being “spin-like” [Fig. 3(c)] to being “charge-like” [Fig. 3(d)]. We expect that the relative strength of the two modes can be determined by studying the $H$-dependence of the LDOS and from the form of the spin-resolved LDOS.

The pairbreaking nature of impurities in $d_{x^2-y^2}$-wave superconductors leads to the suppression of the SCOP, an effect which is not taken into account in the $T$-matrix approach. To study the relevance of this suppression, we compare the results of the $T$-matrix approach with those of the BdG formalism. In Fig. 4(a) we present the spatial form of the SCOP [see Eq. (7)] in a spin droplet for a system with $N = 60 \times 60$ sites and the same parameters as above. The SCOP is significantly suppressed only near the center of the droplet, and quickly recovers its bulk value within a few lattice spacings from the center. In order to ascertain how the SCOP’s suppression affects the LDOS, we compare in Fig. 4(b) [Fig. 4(c)] the results of the $T$-matrix and BdG approaches for the spin↓ (spin↑) LDOS at $\omega_{cp}$. The LDOS obtained from both approaches is in good qualitative agreement and exhibits the same oscillations characteristic of the antiferromagnetic nature of the droplet. The quantitative differences

![Figure 3](image)

**FIG. 3:** (color online) (a) Total LDOS for a spin droplet at $r = (0,0)$ for several $\tilde{g}_s = g_s \langle S_{imp}^z(H,T) \rangle$ ($U = 1$). (b) Total LDOS for a droplet with $\langle s_z(r), \langle \delta n(r) \rangle \neq 0$ and $\alpha = 1/3$. $H_0 \ll H_{ab}^0$ corresponds to $\tilde{g}_s = 100$ meV. Increasing the magnetic field to $2H_0$, ($\tilde{g}_s = 200$ meV) or $4H_0$ ($\tilde{g}_s = 400$ meV) leads to a suppression of the LDOS in the droplet [24]. Since the coupling between impurity and a charge mode is unaffected by the magnetic field, the observation of a magnetic field dependent LDOS as shown in Fig. 3(a) is another direct signature of a static spin droplet.

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are minimal: first, the LDOS of the BdG approach undergoes a $\pi$-phase shift at $\Delta r = 10a_0$ from the center of the droplet, which is absent for the $\hat{T}$-matrix results. Second, the spin-up LDOS of both approaches is out-of-phase at $r = (0, 0)$. A more detailed analysis shows that the latter effect arises from a decrease of the droplet’s effective scattering strength due to the suppression of the SCOP. Since similar good agreement is obtained for a charge droplet, we conclude that the suppression of the SCOP has only minor quantitative effects on the LDOS.

While we considered above a static spin droplet, recent studies [23] suggest that our results remain valid even for $H = 0$ as long as the fluctuation time of the droplet satisfies $\tau_S \gg 1/E_F$. If the spin excitations are sufficiently damped, $\tau_S \rightarrow \infty$ and the droplet becomes static [24]. One might therefore wonder whether signatures of an impurity coupling to a quasi-static mode have already been observed [25]. The effects of collective modes on quasiparticle interference patterns in the fourier-transformed LDOS were discussed in Refs. [17, 26].

Finally, placing an impurity into the CuO$_2$-plane of the HTSC can lead to static lattice distortions. Since such a “phonon droplet” is non-magnetic in nature, it gives rise to a scattering term in Eq. (1) that is identical to that of the charge droplet albeit with a potentially more complicated momentum dependence of $g$. We therefore expect the qualitative effects of static phonon and charge droplets to be quite similar.

In conclusion, we have shown that impurity induced static spin or charge droplets exert qualitatively different effects on the LDOS of a $d_{x^2-y^2}$ superconductor. We find that in a spin droplet, the creation of a resonant impurity state is suppressed, the spin-resolved LDOS exhibits complementary spatial patterns, and a characteristic magnetic field dependence. Since these fingerprints are absent in a charge droplet, our results demonstrate that impurities can be used to identify the nature and relative strength of collective modes not only in the HTSC, but in strongly correlated electron systems in general. We would like to thank J.C. Davis and D. Maslov for helpful discussions and the Aspen Center for Physics for its hospitality. D.K.M. acknowledges financial support by the Alexander von Humboldt Foundation, the NSF under Grant No. DMR-0513415 and the U.S. DOE under Award No. DE-FG02-05ER46225.

FIG. 4: (color online) (a) SCOP along $r = (x, 0)$ for a spin droplet. Inset: intensity plot of the SCOP. (b) Spin-↑ and (c) spin-↓ LDOS of the $\hat{T}$-matrix (red line) and BdG (black line) approaches at $\omega_{sp} = 30$ meV along $r = (x, 0)$.

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