Density of states near a magnetic impurity in the *d*-density wave state

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(Received 19 June 2002; published 28 October 2002)

The response of localized magnetic moments in the pseudogap phase is examined in the *d*-density wave scenario. We find that in the strong scattering limit, the magnetic impurity induces two resonance peaks, one due to the superconducting gap localized at the Fermi energy and another one due to the *d*-density wave gap whose shifting from the Fermi energy is controlled by the chemical potential. The weights of the resonances are proportional with the values of the corresponding gap amplitudes. By measuring the density of states near the magnetic impurity, it is possible to compare our theoretical findings with the available experimental data for probing the existence of the *d*-density wave order in the pseudogap state.

DOI: 10.1103/PhysRevB.66.132509 PACS number(s): 74.20.−z, 74.72.−h, 75.30.Hx

The pseudogap observed in high-temperature superconductors above the superconducting transition temperature T_C has been subject to intense studies in the past years. Influence of the pseudogap formation shows up in different experimental probes, such as nuclear-magnetic-resonance relaxation time, Knight shift, neutron scattering, specific heat, and optical conductivity.[1,2] Recent elastic neutron scattering[3] have found direct evidence for the existence of a new order state, named *d*-density wave (DDW) (Ref. 4) in $YBaCuO_{6+\delta}$. Other experiments[5] are compatible with the DDW scenario.

The principal feature of the DDW state is the existence of the staggered orbital magnetic moments, which breaks time reversal symmetry and translation invariance by one lattice spacing. DDW state competes with the *d*-wave superconductivity (DWS) in the underdoped region of the phase diagram,[6] when the doping is less then critical doped-hole concentration p_{cr}, where the DDW order is believed to vanish. DDW develops below characteristic temperature $T^{\star}$ and is strongly suppressed by the disorder, so only clean samples are expected to show a phase transition at $T^{\star}$. Recently, *c*-axis response and the density of states were investigated in the framework of DDW scenario,[7] and experimental data of Renner *et al.*[8] do not agree with the predictions of the DDW scenario for the quasiparticle density of states. The density of states was also calculated near a nonmagnetic impurity in the same scenario by different authors.[9] It was found that a single resonance peak appears in the local density of states around the impurity, and the position of this resonance peak shifts away from the Fermi surface in accord with the chemical potential. In a similar way, magnetic moments perturb the superconducting properties of the system. When a magnetic impurity is placed in a superconductor, the exchange interaction between the localized impurity spin and the conduction electrons leads to the formation of the Shiba bound states[10] or resonances inside the superconducting gap. Spectral properties of quasiparticle excitations induced by magnetic moments in *d*-wave superconductors were extensively studied using *T*-matrix approximation.[11]

The aim of this paper is to calculate the density of states near a magnetic impurity in a DDW scenario. Such a density of states can be experimentally measured using scanning tunnel microscope (STM) spectroscopy[12] and a direct comparison between the theoretical results and the experimental outcome is possible for probing the existence of the DDW order in the pseudogap state.

The starting point of our analysis is the following Hamiltonian defined by $H=H_0+H_{imp}$, where H_0 is the mean-field Hamitonian describing the coexistence of the DWS and DDW, and H_{imp} is the contribution due to the magnetic impurity.

$$H_0=\sum_{\mathbf{k},\sigma}(\varepsilon_{\mathbf{k}}-\mu)c^{+}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+\sum_{\mathbf{k}}\Delta_{\mathbf{k}}(c^{+}_{\mathbf{k}\uparrow}c^{+}_{-\mathbf{k}\downarrow}+c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}) + i\sum_{\mathbf{k}}\chi_{\mathbf{k}}c^{+}_{\mathbf{k}+\mathbf{Q}\sigma}c_{\mathbf{k}\sigma} \quad (1)$$

where $\Delta_{\mathbf{k}}$ is the superconducting order parameter and $\chi_{\mathbf{k}}$ is the DDW gap. Both $\Delta_{\mathbf{k}}$ and $\chi_{\mathbf{k}}$ have a $(d_{x^2-y^2})$-wave symmetry, $\Delta_{\mathbf{k}}=2\Delta_0(\cos k_x-\cos k_y)$, $\chi_{\mathbf{k}}=2\chi_0(\cos k_x-\cos k_y)$, and $\varepsilon_{\mathbf{k}}$ is the dispersion relation that (in our model) is given by $\varepsilon_{\mathbf{k}}=-2t(\cos k_x+\cos k_y)$. The chemical potential is denoted by μ, and $c^{+}_{\mathbf{k}\sigma}(c_{\mathbf{k}\sigma})$ are the creation (annihilation) operators. Throughout our calculation we have considered for the hopping integral the value $t=0.25$ eV, so $W=8t$ is the bandwidth. The impurity Hamiltonian can be written as $H_{imp}=J\Sigma_{\mathbf{k},\mathbf{k}'}c^{+}_{\mathbf{k},\alpha}\boldsymbol{\sigma}_{\alpha\beta}c_{\mathbf{k}',\beta}\mathbf{S}$, where J is the exchange coupling, $\boldsymbol{\sigma}$ are the Pauli matrices, and $\mathbf{S}$ is the impurity magnetic moment. The exchange interaction preserves the particle-hole symmetry due to the spin-rotational symmetry. The mean-field Hamiltonian can be written in Nambu formalism[13] $H_0=\Sigma_{\mathbf{k}\in rbz}\Psi^{+}_{\mathbf{k}}A_{\mathbf{k}}\Psi_{\mathbf{k}}$, where $\Psi^{+}_{\mathbf{k}}=(c^{+}_{\mathbf{k}\uparrow},c_{-\mathbf{k}\downarrow},c^{+}_{\mathbf{k}+\mathbf{Q}\uparrow},c_{-\mathbf{k}-\mathbf{Q}\downarrow})$, and the matrix $A_{\mathbf{k}}$ is given by

$$A_{\mathbf{k}}=\begin{pmatrix}\varepsilon_{\mathbf{k}}-\mu & \Delta_{\mathbf{k}} & i\chi_{\mathbf{k}} & 0\\ \Delta_{\mathbf{k}} & -(\varepsilon_{\mathbf{k}}-\mu) & 0 & i\chi_{\mathbf{k}}\\ -i\chi_{\mathbf{k}} & 0 & -(\varepsilon_{\mathbf{k}}+\mu) & -\Delta_{\mathbf{k}}\\ 0 & -i\chi_{\mathbf{k}} & -\Delta_{\mathbf{k}} & \varepsilon_{\mathbf{k}}+\mu\end{pmatrix}, \quad (2)$$

and the interating term can be written as $H_{imp}=\Sigma_{\mathbf{k}\in rbz}\Psi^{+}_{\mathbf{k}}V\tau_0\Psi_{\mathbf{k}}$, where $V=1/2JS$. A local Coulomb interaction can be also considered in the form of $H'_{imp}=\Sigma_{\mathbf{k}\in rbz}\Psi^{+}_{\mathbf{k}}U\tau_3\Psi_{\mathbf{k}}$ and describes a scattering of the conduction electrons on a nonmagnetic impurity.[9] The 4×4 $A_{\mathbf{k}}$

matrix can be exactly diagonalized and the Green's function can be calculated as $G_0(\mathbf{k},i\omega_n)=(i\omega_n-A_\mathbf{k})^{-1}$. A direct calculation gives for the eigenvalues of $A_\mathbf{k}$ the values $\pm E_1(\mathbf{k})$ and $\pm E_2(\mathbf{k})$, where $E_1(\mathbf{k})=[(\sqrt{\varepsilon_\mathbf{k}^2+\chi_\mathbf{k}^2}-\mu)^2+\Delta_\mathbf{k}^2]^{1/2}$ and $E_2(\mathbf{k})=[(\sqrt{\varepsilon_\mathbf{k}^2+\chi_\mathbf{k}^2}+\mu)^2+\Delta_\mathbf{k}^2]^{1/2}$ and the Green's function can be written as

$$G_0(\mathbf{k},i\omega_n)=\frac{1}{D}\begin{pmatrix} G_0^{(11)} & G_0^{(12)} & G_0^{(13)} & G_0^{(14)} \\ G_0^{(21)} & G_0^{(22)} & G_0^{(23)} & G_0^{(24)} \\ G_0^{(31)} & G_0^{(32)} & G_0^{(33)} & G_0^{(34)} \\ G_0^{(41)} & G_0^{(42)} & G_0^{(43)} & G_0^{(44)} \end{pmatrix}, \quad (3)$$

where D is the determinant of the $A_\mathbf{k}$ matrix given by $D=[\omega^2-E_1^2(\mathbf{k})][\omega^2-E_2^2(\mathbf{k})]$, and the matrix elements are

$$\begin{aligned}
G_0^{(11)}(\mathbf{k},i\omega_n)&=[\omega+(\varepsilon_\mathbf{k}-\mu)][\omega^2-(\varepsilon_\mathbf{k}+\mu)^2-\Delta_\mathbf{k}^2]\\
&\quad-\chi_\mathbf{k}^2[\omega+(\varepsilon_\mathbf{k}+\mu)],\\
G_0^{(12)}(\mathbf{k},i\omega_n)&=\Delta_\mathbf{k}[\omega^2-(\varepsilon_\mathbf{k}+\mu)^2-\Delta_\mathbf{k}^2]-\Delta_\mathbf{k}\chi_\mathbf{k}^2,\\
G_0^{(13)}(\mathbf{k},i\omega_n)&=i\chi_\mathbf{k}[(\omega-\mu)^2-\varepsilon_\mathbf{k}^2-\Delta_\mathbf{k}^2-\chi_\mathbf{k}^2],\\
G_0^{(14)}(\mathbf{k},i\omega_n)&=2i\Delta_\mathbf{k}\chi_\mathbf{k}\mu,\\
G_0^{(21)}(\mathbf{k},i\omega_n)&=G_0^{(12)}(\mathbf{k},i\omega_n),\\
G_0^{(22)}(\mathbf{k},i\omega_n)&=[\omega-(\varepsilon_\mathbf{k}-\mu)][\omega^2-(\varepsilon_\mathbf{k}+\mu)^2-\Delta_\mathbf{k}^2],\\
&\quad-\chi_\mathbf{k}^2[\omega-(\varepsilon_\mathbf{k}+\mu)],\\
G_0^{(23)}(\mathbf{k},i\omega_n)&=-G_0^{(14)}(\mathbf{k},i\omega_n),\\
G_0^{(24)}(\mathbf{k},i\omega_n)&=i\chi_\mathbf{k}[(\omega+\mu)^2-\varepsilon_\mathbf{k}^2-\Delta_\mathbf{k}^2-\chi_\mathbf{k}^2], \quad (4)\\
G_0^{(31)}(\mathbf{k},i\omega_n)&=-G_0^{(13)}(\mathbf{k},i\omega_n),\\
G_0^{(32)}(\mathbf{k},i\omega_n)&=G_0^{(14)}(\mathbf{k},i\omega_n),\\
G_0^{(33)}(\mathbf{k},i\omega_n)&=[\omega-(\varepsilon_\mathbf{k}+\mu)][\omega^2-(\varepsilon_\mathbf{k}-\mu)^2-\Delta_\mathbf{k}^2]\\
&\quad-\chi_\mathbf{k}^2[\omega-(\varepsilon_\mathbf{k}-\mu)]\\
G_0^{(34)}(\mathbf{k},i\omega_n)&=-\Delta_\mathbf{k}[\omega^2-(\varepsilon_\mathbf{k}-\mu)^2-\Delta_\mathbf{k}^2]+\Delta_\mathbf{k}\chi_\mathbf{k}^2,\\
G_0^{(41)}(\mathbf{k},i\omega_n)&=-G_0^{(14)}(\mathbf{k},i\omega_n),\\
G_0^{(42)}(\mathbf{k},i\omega_n)&=-G_0^{(24)}(\mathbf{k},i\omega_n),\\
G_0^{(43)}(\mathbf{k},i\omega_n)&=G_0^{(34)}(\mathbf{k},i\omega_n),\\
G_0^{(44)}(\mathbf{k},i\omega_n)&=[\omega+(\varepsilon_\mathbf{k}+\mu)][\omega^2-(\varepsilon_\mathbf{k}-\mu)^2-\Delta_\mathbf{k}^2]\\
&\quad-\chi_\mathbf{k}^2[\omega+(\varepsilon_\mathbf{k}-\mu)]
\end{aligned}$$

The mean-field Green's function given by Eqs. (3) and (4) can be used to calculate the physical properties of the system. We are interested in the frequency dependence of the density of states of the bulk system and the modification induced by the presence of a single magnetic impurity.

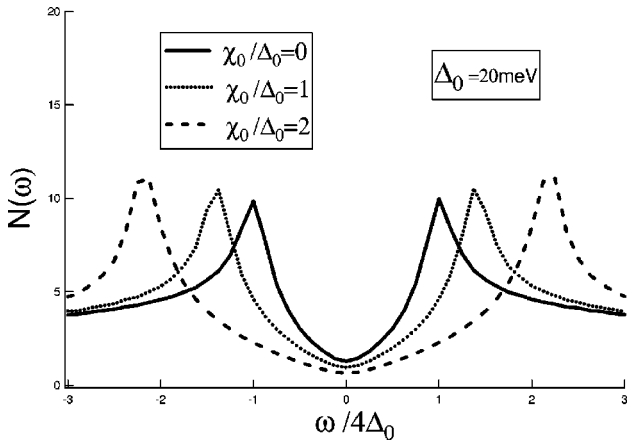

FIG. 1. Density of states for the superconducting state at half filling ($\mu=0$) for different values of the DDW gap.

The density of states for the bulk system can be calculated directly from the mean-field Green's function as $N(\omega)=-2\Sigma_{\mathbf{k}\in rbz}\mathrm{Im}[G_0^{(11)}(\mathbf{k},\omega)+G_0^{(33)}(\mathbf{k},\omega)]$. The results are presented in Fig. 1 for different values of the ratio Δ_0/χ_0. In this case the chemical potential was chosen to be zero ($\mu=0$), so the system is at half filling with perfect electron-hole symmetry. Both the DDW and DWS gaps develop at the Fermi surface, and the system is analogous to the case of a pure DWS with a gap value equal to $\overline{\Delta_\mathbf{k}}=\sqrt{\Delta_\mathbf{k}^2+\chi_\mathbf{k}^2}$.

There is a strong competition between the superconducting gap and the DDW gap in the case where the chemical potential is different from zero, as can be seen from the results for the density of states presented in Fig. 2. Increasing the absolute value of the chemical potential, the superconducting gap remains pinned at the Fermi surface corresponding to ($\omega=0$), while the DDW gap shifts to lower values and develops at energies comparable with the chemical potential, $|\omega|=|\mu|$.

In order to calculate the density of states near a magnetic

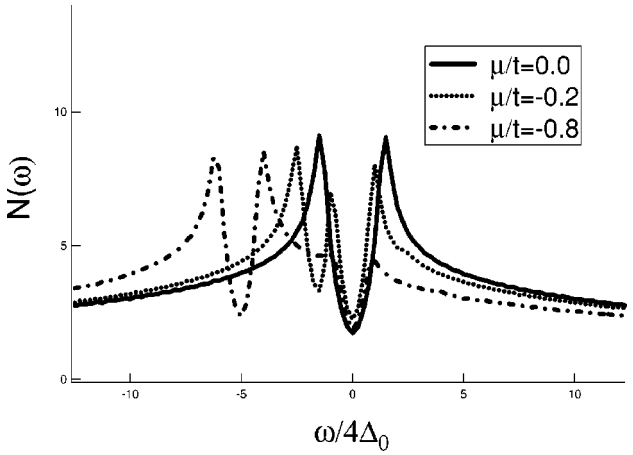

FIG. 2. Density of quasiparticle states for the bulk system for three values of the chemical potential. The Fermi surface corresponds to $\omega=0$. $\Delta_0/\chi_0=1$, $\Delta_0=10$ meV, and $t=0.25$ eV.

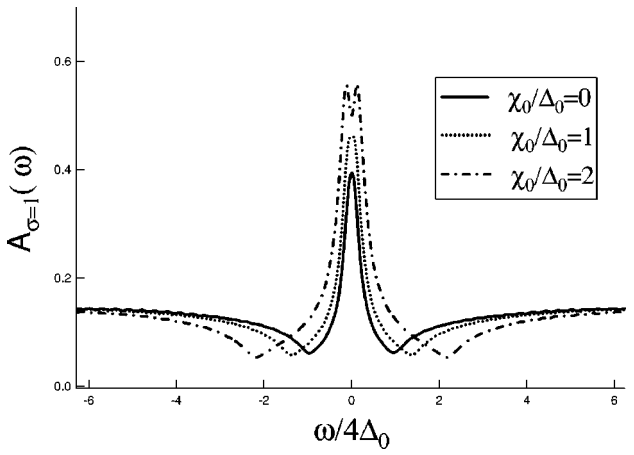

FIG. 3. Spectral density at the impurity site calculated for different ratios of Δ_0/χ_0. The chemical potential is $\mu=0$ (electron-hole symmetry). The other parameters are $\Delta_0=10$ meV, $t=0.25$ eV, $V=30t$, and $U=0.0$.

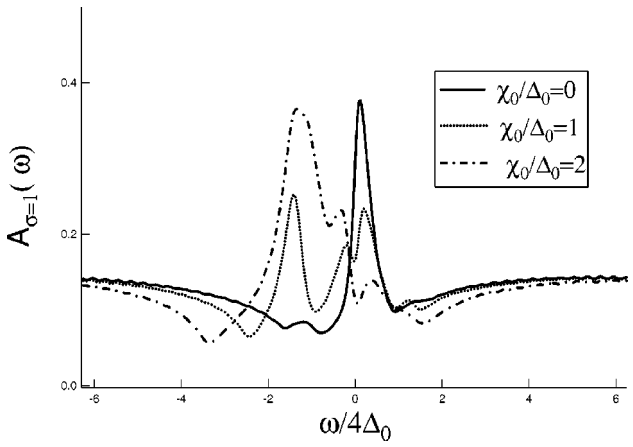

FIG. 4. Same as in Fig. 3 with the chemical potential $\mu=-0.2t$.

moment, we use *T*-matrix formalism and the following approximations: (i) the bulk system is a two-dimensional lattice where a localized magnetic moment is created by a classical spin **S** at $\mathbf{r}=\mathbf{0}$; (ii) the gap function is uniform everywhere and has a $d_{x^2-y^2}$ symmetry.

Multiple scatterings of quasiparticles by the impurity are describe by the *T* matrix, $T(\mathbf{r},\mathbf{r}',\omega)=T(\omega)\delta_{\mathbf{r},0}\delta_{\mathbf{r}',0}$. The presence of magnetic moment modifies the Green's function, and implicitly the physical properties of the system in its neighborhood. The modification in the Green's function depends on the relative position to the magnetic moment as $G(\mathbf{r},\mathbf{r}',\omega)=G_0(\mathbf{r}-\mathbf{r}',\omega)+G_0(\mathbf{r},\omega)T(\omega)G_0(-\mathbf{r}',\omega)$, where $G_0(\mathbf{r},\omega)=N^{-1}\Sigma_{k\in rbz}G_0(\mathbf{k},i\omega_n)e^{i\mathbf{kr}}$ is the Fourier tranform of the Green's function given by the Eq. (3) and *N* is the number of particles in the system. $T(\omega)$ is also a 4×4 matrix that can be calculated as $T(\omega)=[V^{-1}-G_0(\mathbf{r}=0,\omega)]^{-1}$. Impurity bound states or resonances can be identified from the pole structure of the *T* matrix. The bound states correspond to zeros of the determinant $\det[T^{-1}(\omega)]$ for frequencies that satisfy $|\omega|<4\Delta_0$. Zeros in the vicinity of the real axis correspond to resonances. The imaginary part of the *T* matrix poles represent the lifetime of the resonances. We are interested in the density of states exactly at the impurity site in which case the spectral density can be calculated as

$$A_\sigma(\omega)=-1/\pi\mathrm{Im}\left\{\left[\frac{G_0(\omega)}{[1-\sigma(V+\sigma U)G_0(\omega)]}\right]^{(11)}+\left[\frac{G_0(\omega)}{[1-\sigma(V+\sigma U)G_0(\omega)]}\right]^{(33)}\right\} \quad (5)$$

where $G_0(\omega)=G_0(\mathbf{r}=\mathbf{0},\omega)$ and the spin-up (-down) corresponds to the case $\sigma=1(-1)$. The results for the spectral function at the magnetic impurity site are presented in Fig. 3 in the case when the chemical potential is zero (half filling) for different values of the ratio Δ_0/χ_0, as indicated. The resonance at $\omega=0$ in Fig. 3 is fourfold degenerate because of (i) strong magnetic scattering potential that shift the positions of the resonances to $\omega=0$ and (ii) particle-hole symmetry ($\mu=0$) when both DWS gap and DDW gap are opened at the Fermi energy. On increasing the DDW gap value χ_0 the degeneracy starts to rise due to increase of the ratio Δ_0/V, but each resonance still remains doubly degenerate due to the vanishing of the chemical potential.

In Fig. 4 we present the results for the spectral function away from half filling. In the case where $\mu\neq0$ and where DDW gap is zero, the resonance peak is formed at the Fermi energy, and this remains pinned at the Fermi energy for in-band values of the chemical potential ($-4t<\mu<4t$). In contrast, the opening of the DDW pseudogap leads to the formation of a second peak in the density of states at a frequency equal to the chemical potential. When the amplitudes of the DWS and DDW are comparable, the weights of the corresponding resonances are also comparable. On increasing χ_0 the peak becomes dominant and the spectral weight shifts from the DWS peak to the DDW peak. For gap values of $\chi_0\gg\Delta_0$ the DWS peak completely disappears and the only peak that remains corresponds to the DDW gap. An analysis for the modification of the density of states near a nonmagnetic impurity lead to a similar result.[9]

In conclusion, we have calculated the frequency dependence of the density of states of a two-dimensional *d*-wave superconductor in which superconducting order coexists with DDW order. The results for the bulk density of states calculated in this theoretical framework does not agree with the experimental data[8] due to the existence of a second gap at a frequency equal with the chemical potential. We have also calculated the density of states near a magnetic moment in the presence of the DDW order. The spectral density at the magnetic impurity site in the strong scattering limit presents two resonances, one due to the DWS order (localized at the Fermi energy), and the other due to the DDW order shifted in accord with the chemical potential from the Fermi surface. Our results can be directly verified by measuring the density of states near the magnetic moments using STM techniques in the underdoped region of the phase diagram.

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