Marginal Fermi liquid resonance induced by a quantum magnetic impurity in d-wave superconductors

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(March 21, 2022)

We consider a model of an Anderson impurity embedded in a $d_{x^2-y^2}$-wave superconducting state to describe the low-energy excitations of cuprate superconductors doped with a small amount of magnetic impurities. Due to the Dirac-like energy dispersion, a sharp localized resonance above the Fermi energy, showing a marginal Fermi liquid behavior ($\omega \ln \omega$ as $\omega \to 0$), is predicted for the impurity states. The same logarithmic dependence of self-energy and a linear frequency dependence of the relaxation rate are also derived for the conduction electrons, characterizing a new universality class for the strong coupling fixed point. At the resonant energies, the spatial distribution of the electron density of states around the magnetic impurity is calculated, to be confronted with measurements of the scanning tunneling microscopy on Bi$_2$Sr$_2$Ca(Cu$_{1-x}$Ni$_x$)$_3$O$_{8+\delta}$.

PACS numbers:75.20.Hr,71.10.Hf,71.27.+a,71.55.-i

It has been for a long time that non-magnetic and magnetic impurities are exploited to elucidate the microscopic nature of the superconducting state. In the high-$T_c$ cuprates, substitution by divalent metals (Zn and Ni) for Cu in the CuO$_2$ plane offers a particularly important way of introducing such impurities, as they preserve the doping level and introduce only minimal structural disorder. Recently, scanning tunneling microscopy (STM) has been further developed to probe the quasiparticle scattering states around a single Zn impurity in Bi$_2$Sr$_2$Ca(Cu$_{1-x}$Zn$_x$)$_3$O$_{8+\delta}$ with a high spatial and energy resolution by Pan et al. \cite{Pan}. In the obtained STM spectra, an intense zero-bias quasiparticle scattering resonance is found at the Zn sites, and the spatial dependence of the density of states (DOS) in the vicinity of the impurities reveals a fourfold symmetry which characterizes $d_{x^2-y^2}$ wave superconductivity (dSC) \cite{Balatsky}. In fact, the existence of a non-magnetic impurity induced resonant state in dSC was predicted theoretically by Balatsky et al. \cite{Balatsky} earlier.

Here, we consider the scattering effects of magnetic impurities on dSC. In Ni-doped cuprates, in order to maintain the valence of Cu$^{2+}$ ions (3d$^9$, $S=1/2$), the Ni$^{2+}$ ions have a configuration (3d$^8$, $S=1$), and strong antiferromagnetic exchange couplings with the neighboring Cu sites lead to a residual $S=1/2$ on the Ni site, acting as a localized magnetic spin weakly coupled to its environment through exchange interactions \cite{Balatsky}. Although there are some theoretical studies on the quasiparticle states around such a magnetic impurity in dSC state \cite{Balatsky, Balatsky2, Balatsky3}, most of them treated a classical magnetic impurity. It is thus interesting and timing to study how a quantum magnetic impurity affects the quasiparticle states in optimally doped Bi$_2$Sr$_2$Ca(Cu$_{1-x}$Ni$_x$)$_3$O$_{8+\delta}$ superconductors. Since the quantum fluctuations of the internal degrees of freedom of the magnetic impurity play an important role in the ordinary quantum impurity problems, one can thus expect that the effects of a quantum magnetic impurity are significantly different from those of a classical magnetic impurity. Within the slave boson mean field (MF) theory, we predict a sharp resonance above the Fermi level and a marginal Fermi liquid (MFL) behavior for both impurity and surrounding conduction electrons. Moreover, we explicitly calculate the spatial distribution of conduction electron DOS to be compared with STM measurements.

In this Letter, we assume that a BCS-type weak coupling theory is applicable as a phenomenological model for High-$T_c$ optimally doped superconductors though the underlying mechanisms are different. We also assume the magnetic impurities are described by the Anderson model with a strong Hubbard repulsion. When the correlations between the magnetic impurities on different sites are ignored, the model Hamiltonian is given by

$$
\mathcal{H} = \sum_{\kappa\sigma} \epsilon_{\kappa} c_{\kappa\sigma}^{\dagger} c_{\kappa\sigma} + \sum_{\kappa} \Delta_{\kappa} \left( c_{\kappa\uparrow}^{\dagger} c_{-\kappa\downarrow} + h.c. \right) + \epsilon_{d} \sum_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + V \sum_{\k} \left( c_{\k\sigma}^{\dagger} d_{\sigma} + h.c. \right) + U d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}^{\dagger} d_{\downarrow} \right),
$$

where $\epsilon_{k} = \hbar^{2} k^{2} / (2m) - \epsilon_{F}$ is the dispersion of the conduction electrons, $\Delta_{\kappa} = \Delta_{0} \cos 2\phi$ is the dSC order parameter, and $\Delta_{0}$ is the gap amplitude. When Nambu spinors are introduced

$$
\hat{\psi}_{\k} = \begin{pmatrix} c_{\k \uparrow} \\ c_{-\k \downarrow}^{\dagger} \end{pmatrix}, \quad \hat{\phi} = \begin{pmatrix} d_{\uparrow} \\ d_{\downarrow}^{\dagger} \end{pmatrix},
$$

we can simplify the model Hamiltonian in a matrix form

$$
\mathcal{H} = \sum_{\k} \left( \epsilon_{\k} \sigma_{z} + \Delta_{\k} \sigma_{x} \right) \hat{\psi}_{\k} + V \sum_{\k} \left( \hat{\psi}_{\k}^{\dagger} \sigma_{z} \hat{\phi} + h.c. \right) + (\epsilon_{d} + \frac{U}{2}) (\hat{\phi}^{\dagger} \sigma_{z} \hat{\phi} + 1) - \frac{U}{2} (\hat{\phi}^{\dagger} \hat{\phi} - 1)^{2},
$$

as (1).
where $\sigma_z$ and $\sigma_x$ are Pauli matrices. Using the method of equations of motion, the generalized $T$-matrix is derived

$$
\hat{T}(\omega + i0^+) = V \sigma_z \hat{G}_d(\omega + i0^+) \sigma_z \cdot \hat{G}_f(\omega_n),
$$

where $\hat{G}_d(\omega_n) = (i\omega_n - \epsilon_k \sigma_z - \Delta_k \sigma_x)^{-1}$ is the unperturbed Green function (GF) of the conduction electrons. At zero temperature, analytical continuation is used to calculate the perturbed GF through the GF of the impurity: $\hat{G}(r, r'; \omega) = \hat{G}_d(\omega - r' - \omega) + \hat{G}_0(\omega, \omega) \hat{T}(\omega) \hat{G}_d(\omega - r' - \omega)$. The local DOS of the conduction electrons around the magnetic impurity is thus given by

$$
N(r, \omega) = -\frac{1}{\pi} \text{Im} \hat{G}_{11}(\omega, r; r),
$$

and the relaxation rate for the conduction electrons is

$$
\nu(\omega) = \frac{1}{\pi} \text{Im} \hat{G}_{11}(\omega, r; r).
$$

When we take the infinite $U$ limit, the impurity operator is expressed as

$$
\hat{\phi} = (f^+_b b^+ + f^+_f f^+) \text{ in the slave-boson representation,}
$$

where the fermion $f_\sigma$ and the boson $b$ describe the singly occupied and hole states, respectively. The constraint $b^+ b + \sum f^+_\sigma f_\sigma = 1$ has to be imposed. When a MF approximation is applied, the boson operators $b$ and $b^+$ are replaced by a c-number $b_0$, and the constraint is satisfied by introducing a chemical potential $\lambda_0$. Therefore, the MF Hamiltonian is written as

$$
\mathcal{H}_{mf} = \sum_k \hat{\psi}_k^+ (\epsilon_k \sigma_z + \Delta_k \sigma_x) \hat{\psi}_k + \hat{V} \sum_k \left( \hat{\psi}_k^+ \sigma_z \hat{\phi} + h.c. \right) + \epsilon_d \hat{\phi}^+ \sigma_z \hat{\phi} + \epsilon_d + \lambda_0(b_0^2 - 1),
$$

(3)

where $\hat{\phi} = (f^+_b b^+ + f^+_f f^+)$ denotes the Nambu spinors of the impurity quasiparticles and the renormalized parameters $\epsilon_d = \epsilon_d + \lambda_0$ and $\hat{V} = b_0 \hat{V}$.

Using the standard techniques we find $\hat{G}_f(\omega_n) = \left[ i\omega_n - \epsilon_d \sigma_z - \hat{\Sigma}_f(\omega_n) \right]^{-1}$, where the self-energy of the impurity becomes diagonal,

$$
\Sigma_f(\omega_n) = -i\omega_n \sum_k \frac{\hat{V}^2}{\omega_n^2 + \epsilon_k^2 + \Delta_k^2},
$$

(4)

because of the inversion symmetry in the $k$ summation.

At $T = 0$, the ground-state energy change due to impurity is:

$$
\mathcal{E}_{imp} = \epsilon_d + \lambda_0(b_0^2 - 1) - \frac{1}{\pi} \int_0^W d\omega \ln \left[ \omega^2 (1 + \alpha(\omega))^2 + \epsilon_d^2 \right],
$$

where $W$ is the band width and

$$
\alpha(\omega) = \sum_k \frac{\hat{V}^2}{\omega^2 + \epsilon_k^2 + \Delta_k^2}.
$$

The saddle-point equations are derived as

$$
\lambda_0 = \frac{1}{\pi} \int_0^W d\omega \frac{2\omega^2 (1 + \alpha(\omega)) \alpha(\omega)}{\left[ \omega^2 (1 + \alpha(\omega))^2 + \epsilon_d^2 \right] b_0^2},
$$

(5)

$$
b_0^2 = \frac{1}{\pi} \int_0^W d\omega \frac{2\epsilon_d}{\left[ \omega^2 (1 + \alpha(\omega))^2 + \epsilon_d^2 \right]},
$$

(6)

Solving these equations yields $b_0$ and $\lambda_0$ for given parameters $W$, $\Delta_0$, $\Gamma = \pi N_F V^2$, and $\epsilon_d$, where $N_F$ is the DOS at the Fermi surface. In the following, we will choose $\Delta_0$ as the energy unit, $W/\Delta_0 = 20$, and $\Gamma/\Delta_0 = 0.2$.

In the present model the local DOS of quasiparticles near the Fermi surface goes to zero linearly, so the usual logarithmic Kondo singularity in the scattering matrix of the magnetic moment with conduction electrons is thus absent. When $\epsilon_d$ is less than a threshold value, $b_0^2$ is zero, leading to a decoupled free local magnetic moment, namely, no Kondo effect occurs. However, above the threshold value of $\epsilon_d$, $b_0^2$ rises steeply, and then saturates quickly. The usual broad mixed valence regime shrinks to a very narrow regime. In Fig. 1, the ground state phase diagram is calculated in the $\epsilon_d - \Gamma$ plane. For a given value of $\epsilon_d$, there will be a phase transition from the decoupled free spin to the mixed valence, and finally a crossover to the strong coupling regime. The finite threshold value of the phase transition is delineated by the solid line between area I and II, and turns out to be linear in $|\epsilon_d|/\Delta_0$, approximately.

In the mixed valence and strong coupling regimes, the impurity DOS versus $\epsilon_d$ is plotted in Fig. 2. A sharp local resonance always appears above the Fermi energy for each value of $\epsilon_d$, while the corresponding DOS for $\omega < 0$ is broad and small. This is one of the most important differences between the magnetic and non-magnetic impurities scatterings, as the localized resonance always occurs below the Fermi energy for the repulsive potential scattering in the latter case. To the logarithmic accuracy, the zero of the denominator of $\hat{G}_f(\omega_n)$ is given by $\Omega = \Omega' - i\Omega''$, and

$$
\Omega' \approx \epsilon_d \left[ 1 - \frac{2\Gamma}{\pi \Delta_0} \ln \frac{4\Delta_0}{\epsilon_d} \right],
\Omega'' \approx \Omega'' b_0^2 \left( \frac{\Gamma}{\Delta_0} \right),
$$

where $\Omega'$ represents the position of the quasi-particle resonance, while $\Omega''$ corresponds to its width or the inverse lifetime. If the self-energy $\Sigma_f(\omega)$ is expanded near the resonant energy, the impurity DOS can be approximately written in a Lorentzian form $N_{imp}(\omega) \approx \frac{1}{\pi} \frac{b_0^2 \Omega''}{(\omega - \Omega')^2 + (\Omega'')^2}$. At the resonant energy $\omega = \Omega'$, the height of the resonance is $\frac{b_0^2 \Omega''}{(\Omega')^2}$, inversely proportional to the resonant energy. As $\epsilon_d \rightarrow 0$, this resonance becomes arbitrarily sharp and close to the Fermi surface, but the DOS at the Fermi energy is always suppressed to zero for all values of $\epsilon_d$ because of the imaginary part of the impurity self-energy.

Actually, an analytic expression for the retarded self-energy of the magnetic impurity can be derived,

$$
\Sigma_f(\omega) = -\frac{b_0^2}{\pi \Delta_0} \left( \frac{2\Gamma}{\pi \Delta_0} \right) \omega \left[ K \sqrt{1 - \epsilon^2} + i \text{sgn}(\omega) K (\epsilon) \right],
$$

for $\epsilon \equiv |\omega|/\Delta_0 < 1$. Here, $K$ is the complete elliptic integral of the first kind. As $\omega \rightarrow 0$, we have

$$
\text{Re} \Sigma_f(\omega) \sim -b_0^2 \left( \frac{2\Gamma}{\pi \Delta_0} \right) \omega \ln \frac{4\Delta_0}{|\omega|},
$$

(7)
\[ \text{Im } \Sigma_f (\omega) \sim -b_0^2 \frac{\Gamma}{\Delta_0} \left( |\omega| + \frac{1}{4} |\omega|^3 \right), \quad (8) \]

\[ i.e. \text{ precisely } \text{ the MFL behavior proposed by Varma et al. to describe the anomalous normal state properties of optimally doped cuprates [11]. Within the } T \text{- matrix approximation, the self-energy of the conduction electron has exactly the same type of singular behavior. To our knowledge, it is the first time to obtain such a result.} \]

Earlier, the Kondo effect in “gapless” fermion systems (with DOS \( \rho(\epsilon) \sim |\epsilon|^r, 0 < r \leq 1 \)) has been studied by a number of authors [13]. They found a critical value for the Kondo coupling constant below which the local moment decouples. This feature has been reconfirmed in our calculations. However, beyond the critical value they found the same Fermi liquid strong coupling fixed point as in the standard Kondo problem. To the contrary, some dramatically different results are obtained in our studies. We find a MFL behavior in the mixed valence and nearly empty orbital regimes. Namely, the real part of the self-energy goes like \( \omega \ln \omega \), while the imaginary part behaves like \( |\omega| \) as \( \omega \to 0 \). We believe a new universality class for the strong coupling fixed point has been found. The discrepancy with earlier treatments is due to the fact that different limits are considered. In their case the occupation of the impurity is always one and there is a true localized energy level well below the Fermi energy. We, in contrast, are considering the opposite limit, when the hybridization is assumed to be large and the impurity energy levels can merge with the conduction electrons. From the theoretical point of view, the appearance of MFL behavior in our model is fully understandable. It is well-known that near the nodes of a dSC, a Dirac type spectrum appears and the standard dimensional analysis of the quantum field theory can be applied [13]. The scaling dimensions of the Nambu spinors \( \Psi(r, t) \) and \( \phi(t) \) turn out to be -1 and 0 in length units, respectively. Thus short-range interactions between the conduction electrons are irrelevant, while the hybridization term of the Anderson Hamiltonian is marginal and is responsible for this MFL behavior. It seems to us that the Dirac structure of the energy dispersion itself is the main reason behind the MFL for the strong coupling fixed point.

Focus now on \( N(r, \omega) \) in the spatial range \( 0 < r \leq \xi \). Here \( \xi = h \nu F/\Delta_0 \) is the coherence length of dSC state, and also the natural length unit of our model, while in high \( T_c \) dSC state, \( \xi \) is about 10\( \AA \), or roughly 3 lattice spacings. In Fig. 3, the local DOS vs frequency is shown for \( r=0.07\xi \) from the magnetic impurity along the directions of the gap maxima and the gap nodes. In addition to usual V-shape structure, there are quasiparticle resonances near the Fermi energy, and the positions of these resonant peaks coincide with those of the impurity resonances \( \omega = \pm \Omega' \). Along the directions of the gap maxima, there are two resonances below and above the Fermi energy, which are slightly asymmetric in the line shape. On the other hand, along the directions of the gap nodes, there is only one sharp resonance and the local DOS is entirely hole-like. As the impurity energy level \( \epsilon_d \) increases, the quasiparticle resonances become broader, exhibiting a similar dependence as the local resonance of the impurity [6].

We also calculate the spatial variation of the DOS of the conduction electrons. The DOS around the magnetic impurity at the resonance energies is displayed in Fig.4a for \( +\Omega' \) and in Fig.4b for \( -\Omega' \) as a function of spatial variables for \( \epsilon_d/\Delta_0 = -0.2 \) in a logarithmic intensity scale. The quasiparticle resonances induced by the magnetic impurity are highly localized around the impurity, and the spatial oscillation of these resonant states is visible. The largest amplitude of the quasiparticle resonance occurs at the neighborhood of the impurity, and the local electronic structures distinctly differ in Fig.4a and Fig.4b. For \( \omega = +\Omega' \), the local DOS exhibits a four-fold symmetry along the directions of the gap nodes for all distances, consistent with the dSC of the conduction electrons. For \( \omega = -\Omega' \), the local DOS is strongly enhanced in the gap maxima directions at distances \( r \ll \xi \). Further away from the impurity \( (r=\xi) \), it is confined to the neighborhood of the diagonal directions, leading to an eight-fold symmetry.

The logarithmic correction to the real part of the self-energy is a very subtle effect to detect experimentally. However, its imaginary part, the inverse quasiparticle lifetime \( r^{-1} \propto -(V/\epsilon_d)^2 \text{Im } \Sigma_f(\omega) \propto |\omega| \) can be checked by experiments directly. Amazingly, such a linear frequency dependence of the inverse quasiparticle lifetime has been observed in the recent angle-resolved photoemission experiments in optimally doped Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\) along the nodal directions [14,12]. Although these high \( T_c \) cuprates are believed to contain a small number of intrinsic defects or implications and “impurity scatterings” may lead to localization of quasiparticle states, it is not clear whether the Anderson impurity model embedded in dSC state is applicable in this case.

To conclude, we have investigated the quantum magnetic impurity effects in high-\( T_c \) superconductors based on the Anderson model. We have found a new universality class for the strong coupling fixed point for this type of models. We have made explicit predictions on the resonance states around the magnetic impurities to be compared with experiments.

After submitting the manuscript, we received a preprint on optimally doped Bi\(_2\)Sr\(_2\)Ca(Cu\(_{1-x}\)Ni\(_x\))O\(_{8+\delta}\) from Dr. S. H. Pan [13] in which a localized resonance above the Fermi energy has been reported in the DOS of the Ni impurity, and the spatial dependence of the conduction electron DOS at the resonant energies is in a reasonable agreement with our calculations.

One of the authors (G.-M. Zhang) would like to thank D. H. Lee, S. H. Pan, and M. Shaw for their stimulating discussions, and also to acknowledge the financial support from NSF-China (Grant No. 10074036) and the.
Special Fund for Major State Basic Research Projects of China (G2000067107).

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Figures Captions

Fig. 1. The ground-state phase diagram of the model. Three areas denoted by I, II, and III correspond to decoupled local magnetic moment, mixed valence, and strong coupling regimes, respectively.

Fig. 2. The DOS $N_{imp}(\omega)$ of the magnetic impurity, (a) for $\omega < 0$ and (b) for $\omega > 0$, with $\epsilon_d/\Delta_0 = -0.2$, 0.0, 0.2, and 0.4, denoted by solid, dashed, dotted, and dash-dotted lines, respectively.

Fig. 3. The local DOS $N(r, \omega)$ of the conduction electrons for $\epsilon_d/\Delta_0 = -0.2$, 0.0, and 0.2 (from top to bottom) in units of $N_F$. Here $r=0.07\xi$ correspond to the largest amplitude of the quasiparticle resonance at the neighborhood of the impurity. (a) along the directions of the gap maxima and (b) along the directions of the gap nodes.

Fig. 4. The spatial distributions of the conduction electron DOS around the impurity at the resonant energies, (a) $\omega = \Omega'$ and (b) $\omega = -\Omega'$. Here $\epsilon_d/\Delta_0 = -0.2$ and a logarithmic intensity scale is used. The coherent length $\xi$ is about 10Å, or roughly 3 lattice spacings in high $T_c$ cuprates.
(a) $N_{\text{imp}}(\omega)$

(b) $N_{\text{imp}}(\omega)$
(a) $N(r=0.07\xi, \omega) / N_F$

(b) $\omega / \Delta_0$
