Marginal Fermi Liquid Resonance Induced by a Quantum Magnetic Impurity in d-Wave Superconductors

Guang-Ming Zhang,[1,2] Hui Hu,[2] and Lu Yu[3,4]

[1]Center for Advanced Study, Tsinghua University, Beijing 100084, China
[2]Department of Physics, Tsinghua University, Beijing 100084, China
[3]Abdus Salam International Center for Theoretical Physics, P.O. Box 586, Trieste 34100, Italy
[4]Institute of Theoretical Physics, Academic Sinica, Beijing 100080, China

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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. Because of 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 also calculated.

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For a long time nonmagnetic and magnetic impurities have been 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 $Bi_2Sr_2Ca(Cu_{1-x}Zn_x)O_{8+\delta}$ with a high spatial and energy resolution by Pan *et al.* [1]. 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) [1]. In fact, the existence of a nonmagnetic impurity induced resonant state in dSC was predicted theoretically by Balatsky *et al.* [2–4] 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 [5]. Although there are some theoretical studies on the quasiparticle states around such a magnetic impurity in the dSC state [4,6–8], most of them treated a *classical* magnetic impurity. It is thus interesting to study how a *quantum* magnetic impurity affects the quasiparticle states in optimally doped $Bi_2Sr_2Ca(Cu_{1-x}Ni_x)O_{8+\delta}$ 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

$$\begin{aligned}\mathcal{H} &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^+_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} (c^+_{\mathbf{k}\uparrow} c^+_{-\mathbf{k}\downarrow} + \text{H.c.}) \\ &\quad + \epsilon_d \sum_{\sigma} d^+_\sigma d_\sigma \\ &\quad + V \sum_{\mathbf{k}\sigma} (c^+_{\mathbf{k}\sigma} d_\sigma + \text{H.c.}) + U d^+_\uparrow d_\uparrow d^+_\downarrow d_\downarrow, \qquad (1)\end{aligned}$$

where $\epsilon_{\mathbf{k}} = \hbar^2 k^2/(2m) - \epsilon_F$ is the dispersion of the conduction electrons, $\Delta_{\mathbf{k}} = \Delta_0 \cos 2\varphi$ is the dSC order parameter, and Δ_0 is the gap amplitude. When Nambu spinors are introduced

$$\hat{\psi}_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^+_{-\mathbf{k}\downarrow} \end{pmatrix}, \qquad \hat{\varphi} = \begin{pmatrix} d_\uparrow \\ d^+_\downarrow \end{pmatrix},$$

we can simplify the model Hamiltonian in a matrix form

$$\mathcal{H} = \sum_{\mathbf{k}} \hat{\psi}_{\mathbf{k}}^{+}(\epsilon_{\mathbf{k}}\sigma_z + \Delta_{\mathbf{k}}\sigma_x)\hat{\psi}_{\mathbf{k}} + V\sum_{\mathbf{k}}(\hat{\psi}_{\mathbf{k}}^{+}\sigma_z\hat{\varphi} + \text{H.c.}) + \left(\epsilon_d + \frac{U}{2}\right)(\hat{\varphi}^{+}\sigma_z\hat{\varphi} + 1) - \frac{U}{2}(\hat{\varphi}^{+}\hat{\varphi} - 1)^2, \tag{2}$$

where σ_z and σ_x are Pauli matrices. Using the method of equations of motion, the generalized $\mathbf{T}$ matrix is derived $\hat{T}(i\omega_n) = V\sigma_z\hat{G}_d(i\omega_n)V\sigma_z$, with $\hat{G}_{\mathbf{k}}^0(i\omega_n) = (i\omega_n - \epsilon_{\mathbf{k}}\sigma_z - \Delta_{\mathbf{k}}\sigma_x)^{-1}$ 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: $\hat{G}(\mathbf{r},\mathbf{r}';\omega) = \hat{G}^0(\mathbf{r}-\mathbf{r}',\omega) + \hat{G}^0(\mathbf{r},\omega)\hat{T}(\omega)\hat{G}^0(-\mathbf{r}',\omega)$. The local DOS of the conduction electrons around the magnetic impurity is thus given by $N(\mathbf{r},\omega) = -\frac{1}{\pi}\,\text{Im}\hat{G}_{11}(\mathbf{r},\mathbf{r};\omega)$, and the relaxation rate for the conduction electrons is also deduced from $\text{Im}T_{11}(\omega + i0^+)$.

When we take the infinite U limit, the impurity operator is expressed as $\hat{\varphi}^{+} = (f_{\uparrow}^{+}b, f_{\downarrow}b^{+})$ in the slave-boson representation [9,10], where the fermion f_σ and the boson b describe the singly occupied and hole states, respectively. The constraint $b^{+}b + \sum_\sigma f_\sigma^{+}f_\sigma = 1$ 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 λ_0. Therefore, the MF Hamiltonian is written as

$$\mathcal{H}_{\text{mf}} = \sum_{\mathbf{k}} \hat{\psi}_{\mathbf{k}}^{+}(\epsilon_{\mathbf{k}}\sigma_z + \Delta_{\mathbf{k}}\sigma_x)\hat{\psi}_{\mathbf{k}} + \tilde{V}\sum_{\mathbf{k}}(\hat{\psi}_{\mathbf{k}}^{+}\sigma_z\hat{\phi} + \text{H.c.}) + \tilde{\epsilon}_d\hat{\phi}^{+}\sigma_z\hat{\phi} + \tilde{\epsilon}_d + \lambda_0(b_0^2 - 1), \tag{3}$$

where $\hat{\phi}^{+} = (f_{\uparrow}^{+}, f_{\downarrow})$ denotes the Nambu spinors of the impurity quasiparticles and the renormalized parameters $\tilde{\epsilon}_d = \epsilon_d + \lambda_0$ and $\tilde{V} = b_0V$.

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

$$\Sigma_f(i\omega_n) = -i\omega_n\sum_{\mathbf{k}}\frac{\tilde{V}^2}{\omega_n^2 + \epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}, \tag{4}$$

because of the inversion symmetry in the $\mathbf{k}$ summation.

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

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

where W is the bandwidth and $\alpha(\omega) = \sum_{\mathbf{k}}[\tilde{V}^2/(\omega^2 + \epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2)]$. The saddle-point equations are derived as

$$\lambda_0 = \frac{1}{\pi}\int_0^W d\omega\,\frac{2\omega^2[1 + \alpha(\omega)]\alpha(\omega)}{\{\omega^2[1 + \alpha(\omega)]^2 + \tilde{\epsilon}_d^2\}b_0^2}, \tag{5}$$

$$b_0^2 = \frac{1}{\pi}\int_0^W d\omega\,\frac{2\tilde{\epsilon}_d}{\{\omega^2[1 + \alpha(\omega)]^2 + \tilde{\epsilon}_d^2\}}. \tag{6}$$

Solving these equations yields b_0 and λ_0 for given parameters W, Δ_0, $\Gamma = \pi N_F V^2$, and ϵ_d, where N_F is the DOS at the Fermi surface. In the following, we will choose Δ_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 ϵ_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 ϵ_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 ϵ_d-Γ plane. For a given value of ϵ_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 areas 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 ϵ_d is plotted in Fig. 2. A sharp local resonance always appears *above* the Fermi energy for each value of ϵ_d, while the corresponding DOS for $\omega < 0$ is broad and small. This is one of the most important differences between the magnetic and nonmagnetic impurities scatterings, as the localized resonance always occurs *below* the Fermi energy for the repulsive potential scattering in the latter case [2]. To the logarithmic accuracy, the zero of the denominator of $\hat{G}_f(i\omega_n)$ is given by $\Omega = \Omega' - i\Omega''$, and

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

$$\Omega'' \approx \Omega' b_0^2\left(\frac{\Gamma}{\Delta_0}\right),$$

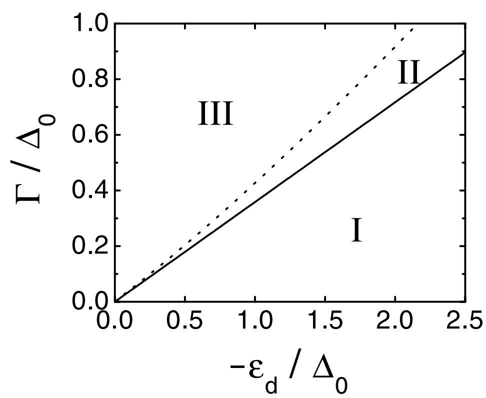

FIG. 1. The ground-state phase diagram of the model. The three areas denoted by I, II, and III correspond to decoupled local magnetic moment, mixed valence, and strong coupling regimes, respectively.

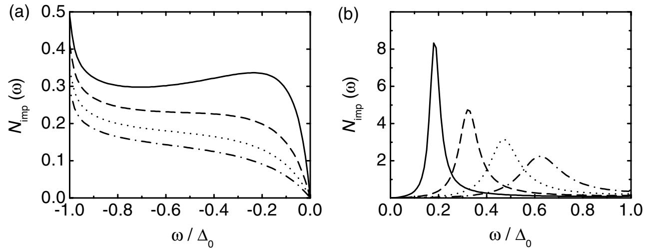

FIG. 2. The DOS $N_{\mathrm{imp}}(\omega)$ of the magnetic impurity, (a) for $\omega < 0$ and (b) for $\omega > 0$, with $\epsilon_d/\Delta_0 = -0.2$, 0.0, 0.2, and 0.4, denoted by solid, dashed, dotted, and dash-dotted lines, respectively.

where Ω' represents the position of the quasiparticle resonance, while Ω'' 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 $N_{\mathrm{imp}}(\omega) \approx \frac{1}{\pi}\{b_0^2\Omega''/[(\omega - \Omega')^2 + (\Omega'')^2]\}$. At the resonant energy $\omega = \Omega'$ the height of the resonance is $\frac{\Delta_0}{\pi\Gamma}\frac{1}{\Omega'}$, inversely proportional to the resonant energy. As $\tilde{\epsilon}_d \to 0$, 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 ϵ_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

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

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

$$\mathrm{Re}\Sigma_f(\omega) \sim -b_0^2\left(\frac{2\Gamma}{\pi\Delta_0}\right)\omega\ln\frac{4\Delta_0}{|\omega|}, \tag{7}$$

$$\mathrm{Im}\Sigma_f(\omega) \sim -b_0^2\frac{\Gamma}{\Delta_0}\left(|\omega| + \frac{1}{4}\frac{|\omega|^3}{\Delta_0^2}\right), \tag{8}$$

i.e., precisely the MFL behavior proposed by Varma *et al.* to describe the anomalous normal state properties of optimally doped cuprates [11]. Within the **T**-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 $\rho(\epsilon) \sim |\rho|^r$, $(0 < r \leq 1)$ has been studied by a number of authors [12]. 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 $\hat{\Psi}(\mathbf{r}, t)$ and $\hat{\phi}(t)$ 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 $N(\mathbf{r}, \omega)$ in the spatial range $0 < \mathbf{r} \leq \xi$. Here $\xi = \hbar v_F/\Delta_0$ is the coherence length of the dSC state, and also the natural length unit of our model, while in the high-T_c dSC state, ξ is about 10 Å, or roughly three 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 the 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

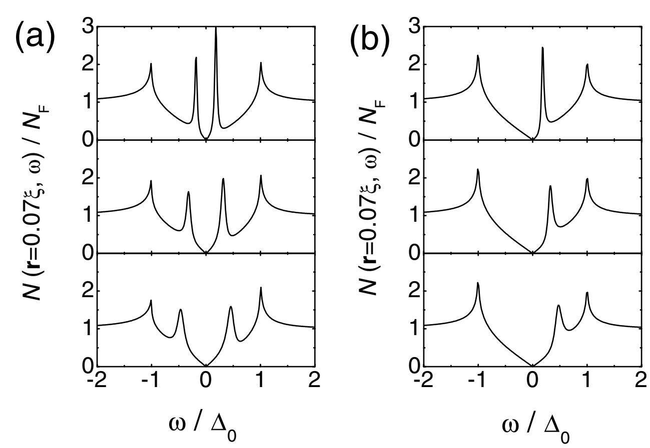

FIG. 3. The local DOS $N(r, \omega)$ of the conduction electrons for $\epsilon_d/\Delta_0 = -0.2$, 0.0, and 0.2 (from top to bottom) in units of N_F. Here $r = 0.07\xi$ corresponds to the largest amplitude of the quasiparticle resonance at the neighborhood of the impurity. (a) Along the directions of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

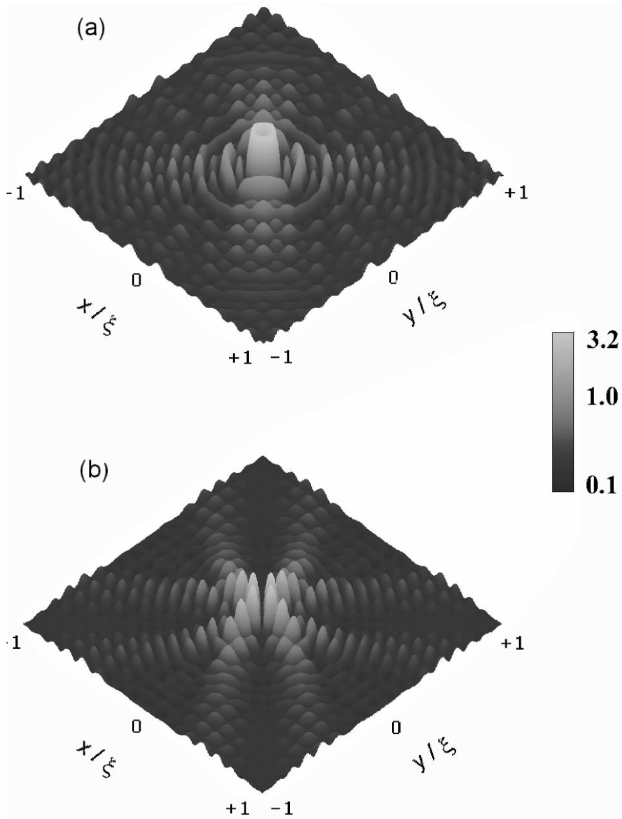

FIG. 4. The spatial distributions of the conduction electron DOS around the impurity at the resonant energies, (a) $\omega = \Omega'$ and (b) $\omega = -\Omega'$. Here $\epsilon_d/\Delta_0 = -0.2$ and a logarithmic intensity scale is used. The coherent length ζ is about 10 Å, or roughly three lattice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

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 holelike. As the impurity energy level ϵ_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 Figs. 4a and 4b. For $\omega = +\Omega'$, the local DOS exhibits a fourfold 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 $r \ll \xi$. Farther away from the impurity ($r \sim \xi$), it is confined to the neighborhood of the diagonal directions, leading to an eightfold 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 $\tau^{-1} \propto -(\tilde{V}/\tilde{\epsilon}_d)^2 \, \mathrm{Im}\Sigma_f(\omega) \propto |\omega|$ 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 $Bi_2Sr_2CaCu_2O_{8+\delta}$ along the nodal directions [14,15]. 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 the 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 model. We have made explicit predictions on the resonance states around the magnetic impurities to be compared with experiments.

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Note added.—After submitting the manuscript, we received a preprint [16] on optimally doped $Bi_2Sr_2Ca(Cu_{1-x}Ni_x)O_{8+\delta}$ 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.

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