Impurity in a d-Wave Superconductor: Kondo Effect and STM Spectra

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(Received 27 July 2000)

We present a theory for recent STM studies of Zn impurities in the superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$, using insights from NMR experiments which show that there is a net $S = 1/2$ moment on the Cu ions near the Zn. We argue that the Kondo spin dynamics of this moment is the origin of the low bias peak in the differential conductance, rather than a resonance in a purely potential scattering model. The spatial and energy dependence of the STM spectra of our model can also fit the experiments.

DOI: 10.1103/PhysRevLett.86.296 PACS numbers: 74.25.Jb, 71.27.+a, 75.20.Hr

Recent progress [1,2] in scanning tunneling microscopy (STM) of surfaces of the high temperature superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ has given us a high resolution probe of its electronic correlations. Especially notable have been studies [1] in the vicinity of Zn impurities on the Cu sites, and the site-specific information on the variation in the pairing correlations. The Zn^{++} ion has spin $S = 0$, and so it appears natural to interpret [1,2] the experiments using a theoretical model [3,4] in which each Zn site acts a potential scatterer of Cu $3d$ electrons forming a d-wave BCS state. However, several key experimental features do not fit easily in this simple picture. There is a large peak in the differential conductance close to zero bias near the Zn site: it is tempting to identify this peak with a quasibound state in the potential scattering model [3], but such a state appears at low energies only for a range of very large potential values depending upon microscopic details [5–7]. Furthermore, the spatial dependence of the zero bias peak is unexpected [8]: it is largest on the Zn site, and with a local maximum on the second neighbor Cu sites [see Fig. 3c in Ref. [1]], and this differs from the general expectations of the potential scattering model [3,4]. Finally, the observed spatially integrated spectrum is asymmetric between positive and negative bias [1], while the potential model predicts approximate symmetry [9].

We shall address these questions here using a rather different theoretical model which was originally motivated by other experiments on Zn or Li impurities (the Li^+ ion is also $S = 0$). A series of beautiful NMR experiments [10–15] have clearly shown that each impurity, despite having no on-site spin, induces a local, unpaired $S = 1/2$ moment on the Cu ions in its vicinity at intermediate energy scales. In the underdoped regime, this can be understood [10,16] by the confining property of the host antiferromagnet, in which the impurity is a localized "holon" which binds the moment of a $S = 1/2$ "spinon." At larger doping, a related picture can be developed by analogy with the theory [17] for moment formation in the disordered metallic state of Si:P—small variations in the potential combine with strong local correlations to induce very localized spin excitations. Other theoretical perspectives [18,19] on local moment formation in the cuprates have also been given. Further evidence for $S = 1/2$ local moments near Zn sites appears from neutron scattering experiments [20]: it has been argued [21] that these are required to explain the strong effects of a small concentration of Zn impurities on a "resonance peak" in the spin dynamic structure factor.

This paper will study a $S = 1/2$ local moment near the Zn/Li site coupled by exchange interactions to the fermionic $S = 1/2$ excitations of a d-wave superconductor. We shall describe the effects of the Kondo screening of the local moment, by the fermionic excitations, on the STM spectra: we shall show that our model leads naturally to a peak in the differential conductance at a low bias of order the Kondo temperature, with a spatial distribution which can fit the experiments. Our spatially integrated spectrum also has a bias asymmetry which increases with decreasing doping.

We begin by describing our model Hamiltonian, $H = H_{\rm BCS} + H_{\rm imp}$, for a single Zn impurity [21]. The first term describes the host superconductor, which we model by a simple BCS Hamiltonian

$$H_{\rm BCS} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger}[(\varepsilon_{\mathbf{k}} - \mu)\tau^z + \Delta_{\mathbf{k}}\tau^x]\Psi_{\mathbf{k}} .$$

Here $\Psi_{\mathbf{k}} = (c_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}^{\dagger})$ is a Nambu spinor at momentum $\mathbf{k} = (k_x, k_y)$ ($c_{\mathbf{k}\alpha}$ annihilates an electron with spin α on a 3D orbital), $\tau^{x,y,z}$ are Pauli matrices in particle-hole space, and μ is a chemical potential. For the kinetic energy, $\varepsilon_{\mathbf{k}}$ we have first (t), second (t'), and third (t'') neighbor hopping, while we assume a d-wave form for the BCS pairing function $\Delta_{\mathbf{k}} = (\Delta_0/2)(\cos k_x - \cos k_y)$. The Zn impurity is at $\mathbf{r} = \mathbf{r}_0$, and is described by

$$H_{\rm imp} = \sum_{\mathbf{r}\in\mathcal{N}} K(\mathbf{r})\vec{S} \cdot c_{\alpha}^{\dagger}(\mathbf{r}) \frac{\vec{\sigma}_{\alpha\beta}}{2} c_{\beta}(\mathbf{r}) + U c_{\alpha}^{\dagger}(\mathbf{r}_0) c_{\alpha}(\mathbf{r}_0) ,$$

where $\sqrt{N_s}\, c_{\alpha}(\mathbf{r}) = \sum_k c_{\mathbf{k}\alpha} e^{i\mathbf{k}\cdot\mathbf{r}}$ (N_s is the number of sites in the lattice) annihilates an electron at site $\mathbf{r}$, $\vec{\sigma}$ are the Pauli matrices in spin space, and $\mathcal{N}$ is a set of sites in the neighborhood of $\mathbf{r}_0$. The spin degree of freedom induced

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by the impurity is represented by the $S = 1/2$ operator $\vec{S}$. The on-site potential scattering of the Zn ion is represented by U: previous analyses of STM spectra of Zn ions [3,4,6] included only this second term in $H_{\rm imp}$ and omitted [9] the degrees of freedom represented by $\vec{S}$. We assume that effects due to spatial variations in the self-consistent pairing amplitude near the impurity, along with those due to Hartree renormalizations from the Coulomb interactions, have been absorbed into the effective parameters $K(\mathbf{r})$ and U (as in [17]); therefore, as the dopant charge carriers are moving in a background of ions that are both doubly charged (Cu^{++} and Zn^{++}), we expect U to be negative and measuring mainly the shift in the d level energy on the Zn (along the same lines, U should be larger and positive for Li^{+} impurities).

An important ingredient in our computation, which influences the spatial form of the STM spectrum, is the $\mathbf{r}$ dependence of the spin-dependent interaction $K(\mathbf{r})$. This is quite difficult to determine from first principles, and we will instead use the spatial information obtained by analyses of Knight shifts in NMR experiments [14,15]. The $S = 1/2$ moment is found to be concentrated on the 4 Cu nearest neighbors of the Zn ion [see Fig. 1(g) in [15] and Fig. 19 in [14]], and the moment on the Zn site itself, $\mathbf{r} = \mathbf{r}_0$, is negligible. We expect that the dopant holes will have a strong preference to reside on a Cu site with a moment (as the Cu spins on the other sites have paired with each other and gained exchange energy); this attraction is realized by $K(\mathbf{r})$, and we take $K(\mathbf{r}) = K_1$ for the 4 sites $\mathbf{r} - \mathbf{r}_0 = (\pm 1, 0), (0, \pm 1)$, while $K(\mathbf{r}_0) = 0$. In principle, it is not difficult to also include the smaller $K(\mathbf{r})$ values at larger values of $|\mathbf{r} - \mathbf{r}_0|$, but we will neglect them here for simplicity. We also note that while the above form for $K(\mathbf{r})$ is reasonable, there is no justification for a corresponding form for the potential scattering term, which is surely largest at $\mathbf{r} = \mathbf{r}_0$, as in $H_{\rm imp}$.

The Kondo effect in H is related to that in a class of models which have been much studied recently [22–24]: these models have a single spin coupled to a fermionic bath whose local density of states, $\rho_\ell(\epsilon)$, vanishes as a power law near the Fermi energy, $\rho_\ell(\epsilon) \sim |\epsilon|^r$, where ϵ is measured from the Fermi level. The usual Kondo effect in a Fermi liquid corresponds to $r = 0$, while the present d-wave superconductor has $r = 1$. The value of r and the presence or absence of particle-hole symmetry [24] play a key role in determining the low energy physics, and a comprehensive phase diagram has been presented by Ingersent and collaborators [24]. For $r = 1$ and with perfect particle-hole symmetry (for H this corresponds to $t' = 0$, $\mu = 0$, and $U = 0$) there is in fact no Kondo effect: the spin is free at low energies for all values of the exchange, K. However, there is a quantum phase transition at a finite magnitude of particle-hole symmetry breaking and at a finite K, to a phase in which the spin is Kondo screened below an energy scale T_K. The universal critical theory for this quantum critical point is not known and we shall not discuss it here.

Here, we shall describe the dynamics of H using a "large N" approach [22,25,26]. While this method has numerous artifacts near the quantum-critical point just mentioned, and is not quantitatively accurate, it does capture the qualitative physics of the Kondo screened phase in an effective manner, and this is our primary interest. We represent the spin $\vec{S}$ by a fermion, f_α, which obeys the constraint $f_\alpha^\dagger f_\alpha = 1$. We impose this by a Lagrange multiplier λ, and decouple the exchange interactions by complex Hubbard-Stratonovich fields $\varphi_{\mathbf{r}}$; λ and $\varphi_{\mathbf{r}}$ are approximated by their static, real saddle point values. The physical quantities are expressed in terms of the Green's function of the Nambu spinor $F = (f_\uparrow, f_\downarrow^\dagger)$, which in Matsubara frequency, ω_n, is $\mathcal{T}(\omega_n) = \langle F(\omega_n) F^\dagger(\omega_n)\rangle$. We have

$$\mathcal{T}^{-1}(\omega_n) = -i\omega_n + \lambda\tau^z - \sum_{\mathbf{r},\mathbf{r}'\in\mathcal{N}} \varphi_{\mathbf{r}}\varphi_{\mathbf{r}'}\tau^z G(\mathbf{r},\mathbf{r}',\omega_n)\tau^z ,$$

where G is the Ψ Green's function with potential scattering alone:

$$G(\mathbf{r},\mathbf{r}',\omega_n) = G^0(\mathbf{r}-\mathbf{r}',\omega_n) - UG^0(\mathbf{r}-\mathbf{r}_0,\omega_n) \times \tau^z\{1 + UG^0[(0,0),\omega_n]\tau^z\}^{-1} \times G^0(\mathbf{r}_0-\mathbf{r}',\omega_n); \quad (1)$$

G^0 is the Green's function of the host, $N_s G^0(\mathbf{r},\omega_n) = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}[-i\omega_n + (\varepsilon_k - \mu)\tau^z + \Delta_k\tau^x]^{-1}$. The values of λ and $\varphi_{\mathbf{r}}$ were obtained by numerically solving the constraint equations $T\sum_{\omega_n} \mathrm{Tr}[\tau^z\mathcal{T}(\omega_n)] = 0$ and $\varphi_{\mathbf{r}} = -[TK(\mathbf{r})/2]\sum_{\omega_n}\sum_{\mathbf{r}'\in\mathcal{N}} \varphi_{\mathbf{r}'}\,\mathrm{Tr}[\tau^z\mathcal{T}(\omega_n) \times \tau^z G(\mathbf{r}',\mathbf{r},\omega_n)]$ (T is the temperature, and Boltzmann's constant $k_B = 1$). Finally, the tunneling density of states (DOS) was obtained as $\mathrm{Im}\,\mathrm{Tr}[\tilde{G}(1+\tau^z)]/2$, where $\tilde{G}$ is the full Ψ Green's function

$$\tilde{G}(\mathbf{r},\mathbf{r}',\omega_n) = G(\mathbf{r},\mathbf{r}',\omega_n) + \sum_{\mathbf{s},\mathbf{s}'\in\mathcal{N}} \varphi_{\mathbf{s}}\varphi_{\mathbf{s}'} G(\mathbf{r},\mathbf{s},\omega_n)\tau^z\mathcal{T}(\omega_n)\tau^z \times G(\mathbf{s}',\mathbf{r}',\omega_n). \quad (2)$$

We now describe our numerical results. For small K_1, the constraint equations have only the solution $\varphi_{\mathbf{r}} = 0$. In the present large N approach, $\vec{S}$ is completely decoupled from the fermions at such a saddle point. This solution corresponds to the free spin phase, and the STM spectra of the large N theory are identical to that of the purely potential scattering model. To include the spin dynamics, we take $K_1 > K_{1c}$ below so that $\varphi_{\mathbf{r}} \neq 0$; we found that the lowest free energy saddle points had a d-wave pattern with $\varphi_{\mathbf{r}} = +[-]\varphi$ for $\mathbf{r} - \mathbf{r}_0 = (\pm 1, 0)\,[(0, \pm 1)]$. Provided particle-hole symmetry is absent, the onset of a nonzero φ corresponds to a phase transition to the Kondo screened phase at K_{1c} (for the particle-hole symmetric case, there is no Kondo screening [24], and the large N equations show that this is so, even for $K_1 > K_{1c}$). The assumption of eventual low energy Kondo screening is also in accord

with indications in NMR [12] and thermodynamic measurements [27]. The large N value for K_{1c} is believed to be an overestimate: this and other shortcomings will be addressed in a forthcoming work employing an alternative "noncrossing approximation" [26].

For $K_1 > K_{1c}$, the energy dependence of the tunneling spectrum is dominated by the form of the scattering matrix $\mathcal{T}(\omega)$; the imaginary part of $\mathcal{T}(\omega)$ shows a pronounced maximum at an energy ω_0 (which becomes a very sharp peak near the Kondo transition), so the location of possible peaks in the local DOS is given by $\pm\omega_0$. On the other hand, $|\omega_0|$ can also be identified with the Kondo temperature, T_K. To see this, consider the local impurity susceptiblity, which is given by $\chi_{\rm loc} = -(T/4)\sum_{\omega_n} \mathrm{Tr}[\mathcal{T}(\omega_n)^2]$. Assuming the simple pole structure $\mathcal{T}(\omega_n) = (-i\omega_n + \omega_0\tau^z)^{-1}$ it is evident that $\chi_{\rm loc}$ changes its character at a T of order $|\omega_0| \sim T_K$.

We show in Fig. 1 the energy and spatial dependence of the local DOS of H for a typical set of parameters at 14% hole doping.

Most significant is the pronounced peak at $\mathbf{r}_0$ (on the Zn site) at a bias, $\omega = -\omega_0$. This was a robust feature of our results: the peak retained a small negative bias and width for a wide range of $K_1 > K_{1c}$ and $U < 0$. Away from the central site, the peaks were much weaker, and varied slightly depending upon U and doping: for -0.4 eV $< U < 0$ at optimal doping (and more robustly at lower doping) we obtained the alternating intensity pattern in Fig. 1(b) [28]. The spatial integral of the spectrum at negative bias is larger than that at positive bias, and the ratio is quoted in Fig. 1. For comparison we show in Fig. 2 the analogous results for a purely potential scattering model [3] ($K_1 = 0$ and $\vec{S}$ absent), where we see dramatically different features. Now the largest peak is on the first neighbors [3]; notice also the change in the color scale in Fig. 2, and that this peak is not as pronounced as the Zn site peak in Fig. 1. Further, we had to choose a very large value of $|U|$ to make the peak sharp and at a small negative bias. Both these features are sensitive to variations in the values of the doping [6], the band structure (t'/t, t''/t) and U: it is not difficult to find broader peaks at higher energies, and to switch the largest peak to positive bias.

We make a few remarks on the spatial dependencies in Fig. 1. The dominant contribution at peak energy comes from the second term on the right hand side of (2), and both the normal (τ^z) and anomalous (τ^x) components of G are largest for sites on opposite sublattices. Using the location of the four sites in $\mathcal{N}$ and the d-wave structure of both the superconducting gap function $\Delta_{\mathbf{k}}$ and the $\varphi_{\mathbf{r}}$ fields, we see that at $\mathbf{r}_0$ the normal (anomalous) Green's functions destructively (constructively) interfere leading to a large peak at $-\omega_0$. This interference is also responsible for the asymmetry of the spatially integrated spectrum. (We note that for an s-wave pattern in the $\varphi_{\mathbf{r}}$ fields the interference mechanism is similar, with the difference that the peak at $\mathbf{r}_0$ appears at $+\omega_0$.) An analogous discussion [3] can be applied to Fig. 2, where

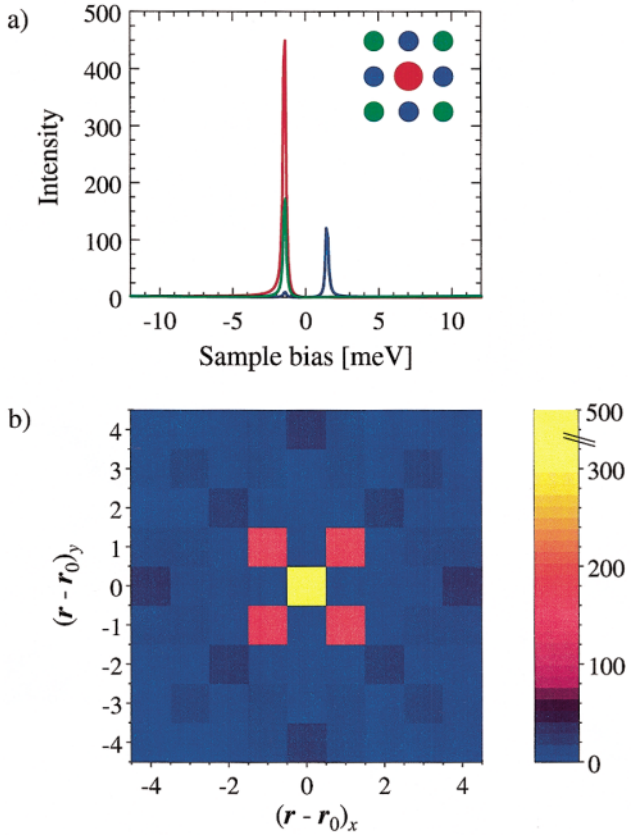

FIG. 1 (color). Calculated tunneling density of states for the Kondo impurity model $H = H_{\rm BCS} + H_{\rm imp}$ at 14% hole doping with a realistic band structure ($t = 0.1$ eV, $t' = -t/4$, $t'' = t/8$), $\Delta_0 = 0.04$ eV, $K_1 = 0.21$ eV, $\mu = -0.09$ eV, and $U = -0.05$ eV. For these parameters $K_{1c} = 0.1$ eV. (a) Tunneling spectrum versus sample bias for the impurity site (red) and the nearest (blue) and second (green) neighbor sites. (b) Spatial dependence of the differential conductance at the bias $\omega = -1.9$ meV ($= -\omega_0$). The ratio of the spatial integrals at $\pm\omega$ is 1.5, and this value increases with decreasing doping.

interference of scattering from different $\mathbf{r}$ is absent. We also note that the coherence peaks, appearing in the DOS at the gap energy, are much suppressed at the impurity site and its neighbors, although we did *not* include a spatial variation of the pairing amplitude. Furthermore, upon moving to the metallic state by setting $\Delta_0 = 0$, our approach is closely related to that of [29], and then the large DOS around the Fermi level leads to a Fano line shape.

To summarize, this paper has introduced a new model ($H = H_{\rm BCS} + H_{\rm imp}$) for STM spectra of Zn/Li impurities in the high temperature superconductors. The model appears to be required to explain NMR [10–15] and neutron scattering measurements [20,21] on the same system. It is therefore satisfying that our model also leads to a low bias peak in the STM: the measured bias of this peak (1.5 meV) suggests that the Kondo screening of the moment (as can be measured directly in NMR) occurs at a temperature of order 15 K.

We conclude by noting related issues: (i) Our model admits a simple generalization to Ni impurities. The Ni^{++}

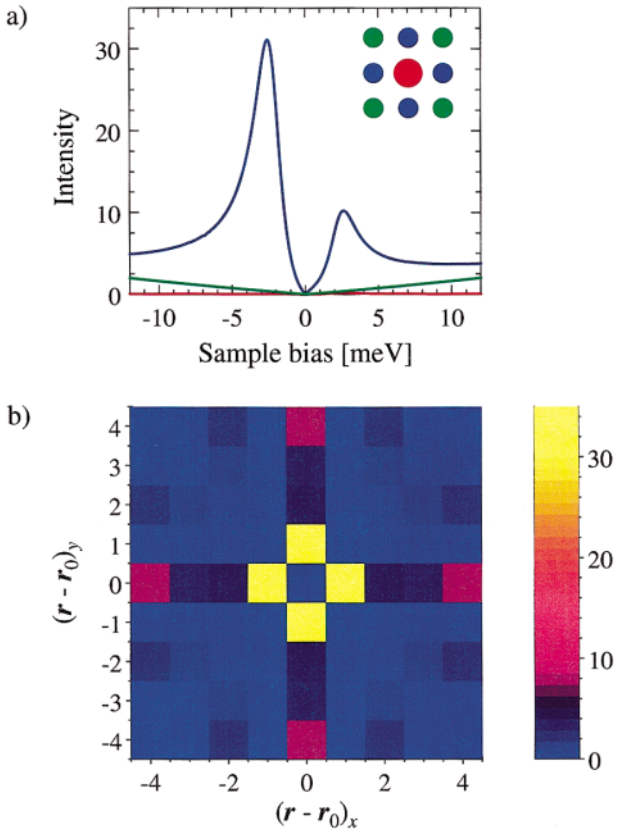

FIG. 2 (color). Parameters as in Fig. 1, but for a purely potential scattering model ($H_{\rm imp}$ has $K_1 = 0$ and no $\vec{S}$) with $U = -4$ eV. The very large $|U|$ is necessary for a low bias peak. The ratio of the spatial integrals at $\pm\omega_0$ is now 1.05, and this value remains around unity with decreasing doping.

ion has $S = 1$, and so we add an additional $S = 1$ degree of freedom $\vec{S}_{\rm Ni}$. A simple choice for a Hamiltonian is $H + K'\vec{S}_{\rm Ni} \cdot \vec{S}$. Depending upon the values of K' and $K(\mathbf{r})$, a rich variety of behaviors appear possible. A likely possibility, suggested by the NMR experiments [13], is that $\vec{S}$ and $\vec{S}_{\rm Ni}$ combine to form a $S = 1/2$ moment; the Kondo coupling of this effective moment is expected to be ferromagnetic [19]—so a $S = 1/2$ moment remains unscreened. The STM spectra will interpolate between the results described here, and those in the presence of a static local magnetic field [30], and this appears to be the case [31]. (ii) In a recent study [21] of the broadening of the collective spin resonance mode [20] by Zn impurities, the Kondo screening of $\vec{S}$ by the fermionic quasiparticles was neglected. This is valid as long as the energy of the resonance mode, $\Delta_{\rm res} \approx 40$ meV, is larger than T_K; this condition is obeyed by the T_K values discussed above.

We thank H. Alloul, W. Atkinson, A. Balatsky, S. Davis, G. Khaliullin, A. MacDonald, and S. Pan for valuable discussions, and U.S. NSF Grant No. DMR 96-23181 and the DFG (VO 794/1-1) for support.

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