The Resonance Peak in Cuprate Superconductors

Dirk K. Morr[1] and David Pines[1,2]
[1]Loomis Laboratory of Physics, University of Illinois at Urbana-Champaign, 1110 W. Green Street, Urbana, Illinois 61801
[2]Center for Materials Science, LANSCE, and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
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We pursue the consequences of a theory in which the resonance peak observed in inelastic neutron scattering experiments on underdoped and optimally doped $YBa_2Cu_3O_{6+x}$ compounds arises from a spin-wave excitation. We find that it is heavily damped in the normal state and only becomes visible in the superconducting state due to the drastic decrease in spin damping. We show that a spin-fermion model correctly describes the doping dependence of the peak position and of the integrated intensity. Finally, we make several predictions concerning resonance peaks in other cuprate superconductors. [S0031-9007(98)06740-4]

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Recent inelastic neutron scattering (INS) experiments have shown that the sharp magnetic collective mode ("resonance peak"), first observed in the superconducting state of $YBa_2Cu_3O_7$ [1], also exists in the underdoped $YBa_2Cu_3O_{6+x}$ compounds [2–7]. As the doping decreases ω_{res}, the peak frequency decreases [2–7], while both the peak width in frequency space and its integrated intensity increase [4,5]. In the underdoped systems, a considerably broadened peak at ω_{res} is also observed in the normal state [4,6]. Fong *et al.* also found that ω_{res} shifts to higher frequencies with decreasing temperature in the superconducting state of $YBa_2Cu_3O_7$ [8].

These new results put tight restrictions on the theoretical scenarios proposed after the discovery of the resonance peak in $YBa_2Cu_3O_7$; these ascribed the resonance peak to a final state interaction between the fermionic particles [9], band structure anomalies [10], interlayer tunneling [11], a new collective mode in the particle-particle channel [12], or a collective spin-wave mode brought about by strong antiferromagnetic correlations [13]. In particular, the observation that ω_{res} decreases with decreasing doping, while the superconducting gap Δ_{SC} is approximately constant, as seen in angle-resolved photoemission spectroscopy (ARPES) [14] and tunneling experiments [15] on Bi2212, contradicts scenarios in which $\omega_{\text{res}} \approx 2\Delta_{\text{SC}}$ [9–11].

In this Letter we use the spin-fermion model to show that the spin-wave scenario, perhaps uniquely, provides a natural explanation for all above-cited experimental results. The dispersion of the spin-wave mode is

$$\omega_q^2 = \Delta_{\text{sw}}^2 + c_{\text{sw}}^2(\mathbf{q} - \mathbf{Q})^2, \tag{1}$$

where Δ_{sw} is the spin-wave gap, c_{sw} is the spin-wave velocity, and $\mathbf{Q} = (\pi, \pi)$. At high temperatures, the mode is strongly damped due to its coupling to planar quasiparticles. In the superconducting state, where the spin damping is minimal, the resonance peak should always be observable provided $\Delta_{\text{sw}} < \omega_c \approx 2\Delta_{\text{SC}}$ [16]. For underdoped systems, at temperatures such that the ARPES [14] experiment shows a leading edge gap in the quasiparticle spectrum, the spin damping present at higher temperatures is reduced sufficiently so that the resonance mode becomes visible. For optimally doped systems with no leading edge gap, the spin mode is overdamped and invisible. In contrast to the results of Refs. [9–11], the existence of the resonance peak is *not* related to the interlayer coupling, and should be observed in single-layer compounds if the superconducting gap is large enough. We consider first the two-layer system $YBa_2Cu_3O_{6+x}$, for which the bonding and antibonding tight-binding quasiparticle bands are given by

$$\epsilon_{\mathbf{k}}^{\pm} = -2t[\cos(k_x) + \cos(k_y)] - 4t' \cos(k_x)\cos(k_y) \pm t_{\perp} - \mu\,, \tag{2}$$

where t, t' are the hopping elements between in-plane-nearest and next-nearest neighbors, respectively, $t_{\perp}$ is the hopping between nearest neighbors on different planes, and μ is the chemical potential. In a spin-fermion model [17], the spin-wave propagator, χ, is given by

$$\chi^{-1} = \chi_0^{-1} - \operatorname{Re}\Pi - i \operatorname{Im}\Pi\,, \tag{3}$$

where χ_0 is the bare propagator, and Π is the irreducible particle-hole bubble.

Since the form of the bare propagator in Eq. (3) is model dependent, and thus somewhat arbitrary, we choose a form for $(\chi_0^{-1} - \operatorname{Re}\Pi)$ which is the lowest order expansion in momentum and frequency of a hydrodynamical form of $\operatorname{Re}\chi^{-1}$ [18] and can be shown to reproduce the INS experiments in the normal state of the underdoped $YBa_2Cu_3O_{6+x}$ compounds [7,19],

$$\chi_0^{-1} - \operatorname{Re}\Pi = \frac{1 + \xi^2(\mathbf{q} - \mathbf{Q})^2 - \omega^2/\Delta_{\text{sw}}^2}{\alpha\xi^2}\,, \tag{4}$$

where ξ is the magnetic correlation length, $\Delta_{\text{sw}} = c_{\text{sw}}/\xi$, and α is an overall constant. We assume that the form of Eq. (4) does not change in the superconducting state. Although Dai *et al.* [3] recently found that, for

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frequencies well below the resonance peak, the peaks in the spin fluctuation spectrum occur at incommensurate positions, which roughly scale with doping, we argue that the use of the commensurate form, Eq. (4), is justified for the description of the resonance peak since (a) no resonance peak has been observed at incommensurate positions, (b) incommensurate structure and the resonance peak are well separated in frequency, and (c) the use of a commensurate instead of an incommensurate form will influence only low-frequency results in the normal state.

With these assumptions, we need calculate only the imaginary part of Π which describes the damping brought about by the decay of a spin excitation into a particle-hole pair. In the odd channel, $\mathrm{Im}\,\Pi$ includes only quasiparticle excitations between the bonding and antibonding bands. In the superconducting state we find, to lowest order in the spin-fermion coupling g_{eff} (for $\omega > 0$),

$$\mathrm{Im}\,\Pi_{\mathrm{odd}} = \frac{3\pi g_{\mathrm{eff}}^2}{8} \sum_{\mathbf{k}} [1 - n_F(E^+_{\mathbf{k+q}}) - n_F(E^-_{\mathbf{k}})]\left[1 - \frac{\epsilon^+_{\mathbf{k+q}}\epsilon^-_{\mathbf{k}} + \Delta_{\mathbf{k+q}}\Delta_{\mathbf{k}}}{E^+_{\mathbf{k+q}}E^-_{\mathbf{k}}}\right]\delta(\omega - E^-_{\mathbf{k}} - E^+_{\mathbf{k+q}}) + [n_F(E^-_{\mathbf{k}}) - n_F(E^+_{\mathbf{k+q}})]\left[1 + \frac{\epsilon^+_{\mathbf{k+q}}\epsilon^-_{\mathbf{k}} + \Delta_{\mathbf{k+q}}\Delta_{\mathbf{k}}}{E^+_{\mathbf{k+q}}E^-_{\mathbf{k}}}\right]\{\delta(\omega + E^-_{\mathbf{k}} - E^+_{\mathbf{k+q}}) - \delta(\omega - E^-_{\mathbf{k}} + E^+_{\mathbf{k+q}})\}, \tag{5}$$

where n_F is the Fermi function, and $E^{\pm}_{\mathbf{k}} = \sqrt{(\epsilon^{\pm}_{\mathbf{k}})^2 + |\Delta_{\mathbf{k}}|^2}$ is the dispersion of the bonding and antibonding bands in the superconducting state, which we assume is described by the d-wave gap $\Delta_{\mathbf{k}} = \Delta_{\mathrm{SC}}[\cos(k_x) - \cos(k_y)]/2$. The normal state result for $\mathrm{Im}\,\Pi_{\mathrm{odd}}$ is recovered with $\Delta_{\mathrm{SC}} = 0$. We determine g_{eff} by requiring that $\mathrm{Im}\,\Pi_{\mathrm{odd}}$ reproduces the spin damping seen at low frequencies in NMR experiments in the normal state of $YBa_2Cu_3O_{6+x}$ [20] and assume that g_{eff} does not change in the superconducting state. It was recently shown [21] that higher order self-energy and vertex corrections lead only to minor changes in $\mathrm{Im}\,\Pi$, which justifies our use of the lowest order process in Eq. (5).

We first discuss our results for $YBa_2Cu_3O_7$, which were obtained with $t = 300$ meV, $t' = -0.40t$, $t_\perp = 0.3t$, $\mu = -1.27t$ (which corresponds to a 22% hole concentration in the planes), and $\Delta_{\mathrm{SC}}(T = 0) \approx 25$ meV, a value extracted from the tunneling experiments of Maggio-Aprile *et al.* [22]. In Fig. 1 we present our result for $\mathrm{Im}\,\Pi_{\mathrm{odd}}$ at $\mathbf{Q} = (\pi, \pi)$ as a function of frequency for the normal (solid line) and superconducting states (dashed line). In the normal state the spin damping increases linearly with frequency, as is to be expected [23]. The spin damping in the superconducting state is characterized by a steplike feature at $\omega_c \approx 2\Delta_{\mathrm{SC}}$ which arises from the creation of a particle-particle pair above the superconducting gap. At $T = 0$, there are no quasiparticle excitations below ω_c, and the spin damping vanishes. The step in $\mathrm{Im}\,\Pi$ will then, via the Kramers-Kronig relation, lead to a logarithmic divergence in $\mathrm{Re}\,\Pi$. This is neglected in Eq. (4), since the inclusion of fermion lifetime effects as found, e.g., in strong coupling scenarios, eliminates the sharp step in $\mathrm{Im}\,\Pi$ and the divergence in $\mathrm{Re}\,\Pi$.

In Fig. 2 we present our results for χ''_{odd} at $\mathbf{Q} = (\pi, \pi)$ as a function of frequency. In the normal state, the spin excitations are overdamped; χ'' exhibits a flat maximum at about $\omega = 20$ meV. In contrast, in the superconducting state the spin damping is so strongly reduced that the spin-wave mode, which is now very sharp in frequency, becomes visible at $\omega_{\mathrm{res}} = \Delta_{\mathrm{sw}}$, which we have chosen to be 41 meV to reproduce the experimentally measured peak. The resulting spin-wave velocity, $c_{\mathrm{sw}} = \xi\Delta_{\mathrm{sw}} \approx 90$ meV is quite reasonable, since $c_{\mathrm{sw}} = 120 \pm 20$ meV in $YBa_2Cu_3O_{6.5}$ and $c_{\mathrm{sw}} = 180$ meV in the undoped compound [7]. Our results can be easily understood using Eq. (4), since the intensity at $\omega = \Delta_{\mathrm{sw}}$ is given by

$$\chi''_{\mathrm{odd}}(\mathbf{Q}, \omega = \Delta_{\mathrm{sw}}) = \{\mathrm{Im}\,\Pi_{\mathrm{odd}}(\mathbf{Q}, \Delta_{\mathrm{sw}})\}^{-1}. \tag{6}$$

If $\Delta_{\mathrm{sw}} < \omega_c$, $\mathrm{Im}\,\Pi_{\mathrm{odd}}$ in the superconducting state is much smaller than in the normal state and, consequently, χ''_{odd} is strongly enhanced at $\omega = \Delta_{\mathrm{sw}}$. Our result is robust against changes in the band parameters, in contrast to some scenarios [9–11].

In the inset in Fig. 2 we plot χ''_{odd} for fixed frequency $\omega = 41$ meV along the $(0,0)$ to (π, π) direction. We

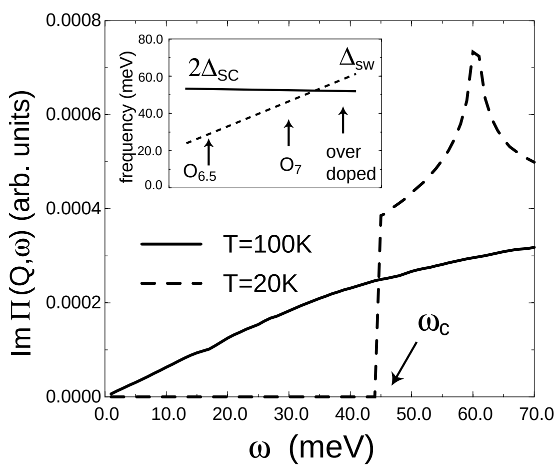

FIG. 1. $\mathrm{Im}\,\Pi_{\mathrm{odd}}$ at $\mathbf{Q} = (\pi, \pi)$ as a function of frequency in the normal state (solid line) and the superconducting state (dashed line). Inset: Schematic doping dependence of Δ_{sw} and $2\Delta_{\mathrm{SC}}$.

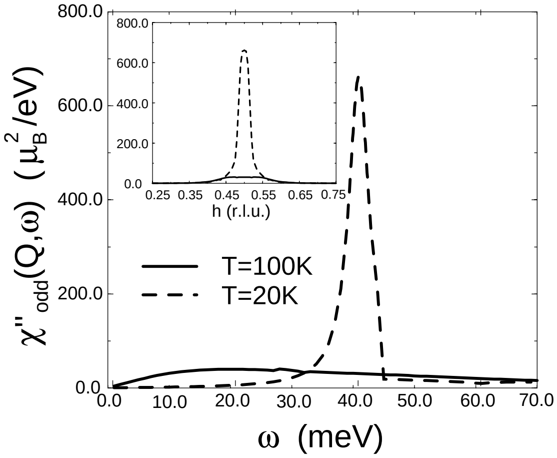

FIG. 2. χ'' at $\mathbf{Q} = (\pi, \pi)$ as a function of frequency in the normal state (solid line) and the superconducting state (dashed line). Inset: χ'' for fixed frequency $\omega = 41$ meV along $q_x = q_y$.

find that the resonance peak is sharp in momentum space, in agreement with the experimental observations [3,8]. The sharpness of the resonance peak in both momentum and frequency space can be easily understood from Eqs. (1) and (4). One expects to find a resonance peak at ω_q which follows the dispersion of the spin excitations, Eq. (1), as long as $\omega_q < 2\Delta_{SC}$. Since in $YBa_2Cu_3O_7$ $\Delta_{sw} \approx 2\Delta_{SC}$, the resonance peak is necessarily confined in both momentum and frequency space. We will show below that this situation is different in the underdoped compounds. Since $\Delta_{sw} \approx 2\Delta_{SC}$ for $YBa_2Cu_3O_7$, we expect $\Delta_{sw} > 2\Delta_{SC}$ for the magnetically overdoped compounds (where $\xi < 2$), and predict that no resonance peak should be observed (see inset in Fig. 1).

Fong *et al.* [8] found that ω_{res} increases slightly between T_c and $T = 10$ K. Since $\Delta_{sw} = c_{sw}/\xi$ in our model, their result implies that ξ decreases over this temperature range, a finding consistent with the changes in the transverse relaxation rate, $T_{2G}^{-1} \sim \xi$, in the superconducting state of $YBa_2Cu_3O_7$ measured by Milling *et al.* [24] who report a decrease of T_{2G}^{-1} by about 10% with decreasing temperature. Put another way, in our model, the results of Milling *et al.* require that ω_{res} increase by some 10% below T_c.

The fact that ω_{res} is determined by the spin gap Δ_{sw} explains the absence of the resonance peak in the even channel of $YBa_2Cu_3O_{6+x}$. For $YBa_2Cu_3O_{6.5}$, Bourges *et al.* [7] found a spin gap, $\Delta_{sw}^{even} = 53$ meV, in the even channel which may be expected to be larger in $YBa_2Cu_3O_7$. Since $\Delta_{sw}^{even} > \omega_c$, the damping of the even spin excitations around $\mathbf{Q} = (\pi, \pi)$ will *not* decrease upon entering the superconducting state and no resonance peak is to be expected.

We consider next the resonance peak in the underdoped $YBa_2Cu_3O_{6+x}$ compounds; our results are summarized in inset (a) of Fig. 3. Fong *et al.* found that ω_{res} decreases to $\omega_{res} = 25$ meV in $YBa_2Cu_3O_{6.5}$ while the integrated intensity of the peak increases from $I_{int} \approx 1.1\mu_B^2$ in $YBa_2Cu_3O_7$ to $I_{int} \approx 2.6\mu_B^2$ in $YBa_2Cu_3O_{6.5}$. In our model, the doping dependence of $\omega_{res} = \Delta_{sw} = c_{sw}/\xi$ is determined by changes in c_{sw} and ξ. From an analysis of NMR [20] and INS experiments [19], we know that $\xi(T_c)$ increases from ≈ 2.2 in $YBa_2Cu_3O_7$ to ≈ 6 in $YBa_2Cu_3O_{6.5}$. This change in ξ more than compensates any increase of c_{sw} as the doping is reduced and so brings about a decrease in Δ_{sw}. Furthermore, Bourges *et al.* [7] found a normal state spin gap in $YBa_2Cu_3O_{6.5}$, $\Delta_{sw} \approx 23$ meV [7], in agreement with the position of the resonance peak in the superconducting state reported by Fong *et al.* [4]. The integrated intensity I_{int} of the resonance peak in the limit $\mathrm{Im}\,\Pi_{odd} \ll 1/\alpha\xi^2$, i.e., for small spin damping, is given by $I_{int} = \alpha\xi^2\Delta_{sw}\pi/4$. For $YBa_2Cu_3O_7$, $\alpha = 15\mu_B^2/\mathrm{eV}$ which yields $I_{int} = (2.3 \pm 0.4)\mu_B^2$. For $YBa_2Cu_3O_{6.5}$, we find from our analysis of INS data in the normal state $\alpha \approx 9\mu_B^2/\mathrm{eV}$, and thus $I_{int} = (6.2 \pm 1.0)\mu_B^2$. Both values for I_{int} are a factor of 2 larger than the values measured experimentally by Keimer *et al.* [5]; however, the relative increase of I_{int} on going from $YBa_2Cu_3O_7$ to $YBa_2Cu_3O_{6.5}$ is in quantitative agreement with their results.

As $2\Delta_{SC}$ and Δ_{sw} become well separated in the underdoped compounds [14,15], we predict a resonance peak for momenta in a region around $\mathbf{Q}$ which is determined by $\omega_q < \omega_c$ [see inset (b) of Fig. 3]. In Fig. 3 we show how the resonance peak shifts to higher frequencies when one moves in momentum space from $\mathbf{Q} = (\pi, \pi)$ to $\mathbf{q} = 0.97(\pi, \pi)$. Because of the limited momentum resolution of INS experiments, we do not expect that these peaks can be resolved; this implies that one should observe only one broad peak which extends from Δ_{sw} up to ω_c. This broadening of the peak width is just what is observed by Fong *et al.* [4] in $YBa_2Cu_3O_{6.5}$ and $YBa_2Cu_3O_{6.7}$.

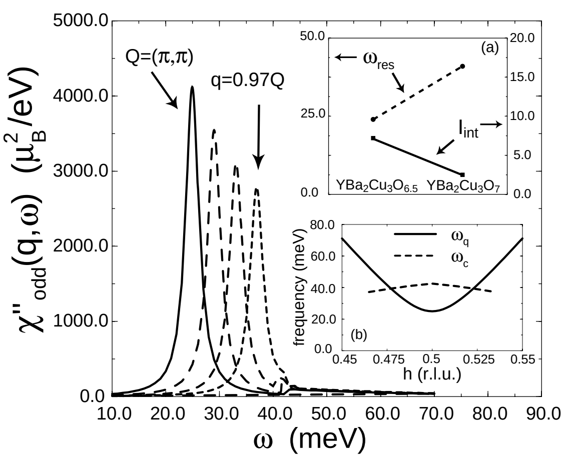

FIG. 3. The resonance peak for momenta in the vicinity of $\mathbf{Q} = (\pi, \pi)$. Inset (a): The doping dependence of ω_{res} (in meV, dashed line) and I_{int} (in μ_B^2, solid line). Inset (b): Spin excitation spectrum and ω_c along $q_x = q_y$.

For the underdoped compounds, two groups found a precursor of the resonance peak in the normal state below $T_* \approx 200$ K, in the so-called strong pseudogap region [4,7]. At the same time, ARPES experiments found that, below T_*, the low-frequency spectral weight of the "hot" fermionic quasiparticles around $(0, \pi)$ is suppressed (the "leading-edge gap") [14], which immediately leads to a decrease of the spin damping at $\mathbf{Q} = (\pi, \pi)$ and an enhancement of χ''_{odd}. Our model thus predicts an enhancement of χ''_{odd} around ω_{res} in the normal state of those superconductors for which a leading-edge gap occurs below T_*.

It follows from the above analysis that a resonance peak should occur in all cuprate superconductors for which the condition $\Delta_{\mathrm{sw}} < 2\Delta_{\mathrm{SC}}$ is satisfied. This implies that the resonance peak is *not* directly related to the bilayer structure of $YBa_2Cu_3O_{6+x}$. In $La_{2-x}Sr_xCuO_4$, where $\Delta_{\mathrm{SC}} \approx 9$ meV and $\Delta_{\mathrm{sw}} > 25$ meV [25], the above condition is not satisfied and, consequently, no resonance peak is to be expected. On the other hand, for the single-layer material $HgBa_2CuO_{4+\delta}$ with an optimum $T_c = 95$ K, we expect Δ_{SC} to be comparable to that found in $YBa_2Cu_3O_7$, so that it is a good candidate for the observation of a resonance peak.

Our model also provides a natural explanation for the results of recent INS experiments on Zn-doped $YBa_2Cu_3O_{6.97}$ [26]. A Zn concentration of 2% which suppresses T_c to 69 K completely destroys the resonance peak in the superconducting state, and generates a significant amount of spectral weight in χ'' at low frequencies. Since $\Delta_{\mathrm{sw}} \approx 2\Delta_{\mathrm{SC}}$ in this material, to the extent that Δ_{sw} is not markedly influenced by Zn, a quite modest Zn-induced decrease in Δ_{SC} will render the resonance unobservable in the superconducting state. For the underdoped compounds, on the other hand, since Δ_{sw} and $2\Delta_{\mathrm{SC}}$ are more clearly separated, a larger amount of Zn would be required to suppress the resonance. The appearance of low-frequency spectral weight in χ'' shows that a considerable spin damping persists in the superconducting state, as might be expected from Zn-induced changes in the low-frequency spectral weight in the single-particle spectrum.

In summary, we have shown that a spin-wave model provides a natural explanation for the doping and temperature dependence of the existing INS experiments on the appearance of a resonance peak in the superconducting state and of a resonance feature in the normal state of underdoped systems. We proposed necessary conditions for the observation of the peaks and resonance features, and so explain the failure to observe either of them in $La_{2-x}Sr_xCuO_4$. We argue that the occurrence of the resonance peak is not directly related to the bilayer structure of $YBa_2Cu_3O_{6+x}$, and predict that it should also be observable in single-layer cuprates with a sufficiently large superconducting gap.

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