

Slave Boson Approach to Neutron Scattering in $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ Superconductors

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The evolution of the so-called “41 meV resonance” in the magnetic response of YBCO cuprates is studied with slave boson theory for the t - t' - J model. The resonance appears as a collective spin fluctuation in the d -wave superconducting (SC) state. It is undamped at optimal doping due to a threshold in the excitation energies of particle-hole pairs with relative wave vector (π, π) . When hole filling is reduced, the resonance moves to lower energies and broadens. Below the resonance energy we find a crossover to an incommensurate response in agreement with a recent experiment on $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$. We show that dynamic nesting in the d -wave SC state causes this effect. [S0031-9007(99)08857-2]

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One of the puzzling phenomena in copper-oxide superconductors is the so-called “41 meV resonance” observed in inelastic neutron-scattering (INS) experiments on optimally doped $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ (YBCO) compounds in the superconducting (SC) phase [1–5]. The magnetic susceptibility $\chi''(\mathbf{q}, \omega)$ shows a peak at the antiferromagnetic (AF) wave vector (π, π) and an energy $\omega_0 = 41$ meV. The peak appears to be resolution limited, i.e., almost undamped, and vanishes above T_c . In underdoped YBCO the peak shifts to lower energies $\omega_0 < 41$ meV [6–8] and develops some damping. It is also visible in the spin-gap regime above T_c . Several theoretical approaches to the magnetic excitations have been proposed [9–15]. In most cases [9–14] the resonance at optimal doping is identified as a collective spin fluctuation, which is stabilized through the suppression of quasiparticle damping in the SC state, and vanishes in the normal phase. The question arises how this mode evolves with decreasing doping. In particular, it is unclear how the finite damping at intermediate doping levels can be obtained, since the peak is expected to narrow and become a spin-wave (Bragg) peak at zero energy when the Néel state is reached. There is also experimental evidence [2,16] that the magnetic response in YBCO at energies somewhat below ω_0 is incommensurate. It is dominated by four peaks at $\mathbf{q} = (\pi, \pi \pm \delta)$ and $\mathbf{q} = (\pi \pm \delta, \pi)$, a pattern previously known only for the $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4+y}$ family of compounds. In view of the new experimental data, we reinvestigate the spin response in slave-boson mean-field theory [9–11], focusing on the evolution of the resonance with hole filling (doping) and the crossover commensurate-incommensurate with variation of energy.

We start from the t - t' - J model for a single CuO_2 layer. Results specific to the bilayer structure of YBCO will be presented elsewhere. The model reads

$$H = - \sum_{(i,j),\sigma} t c_{i\sigma}^\dagger c_{j\sigma} - \sum_{(i,j)',\sigma} t' c_{i\sigma}^\dagger c_{j'\sigma} + \frac{1}{2} \sum_{(i,j)} J \mathbf{S}_i \cdot \mathbf{S}_j.$$

Sums include nearest neighbor (i, j) or next nearest neighbor $(i, j)'$ Cu sites on a 2D square lattice. Physical op-

erators $c_{i\sigma} = b_i^\dagger f_{i\sigma}$, $\mathbf{S}_i = \frac{1}{2} \sum_{\sigma,\sigma'} f_{i\sigma}^\dagger \boldsymbol{\tau}^{\sigma\sigma'} f_{i\sigma'}$ are represented by auxiliary (“slave”) bosons b_i carrying the charge and fermions $f_{i\sigma}$ representing the spin σ . In mean-field theory the d -wave superconducting phase is represented by condensed bosons $b_i \rightarrow \langle b_i \rangle$ and fermions in a d -wave BCS state with dispersion

$$\begin{aligned} \varepsilon(\mathbf{k}) = & -2\tilde{t}[\cos(k_x) + \cos(k_y)] \\ & -4\tilde{t}' \cos(k_x) \cos(k_y) - \mu_f \end{aligned}$$

and gap $\Delta(\mathbf{k}) = \Delta_0[\cos(k_x) - \cos(k_y)]/2$. Renormalized hopping parameters are $\tilde{t} = xt + \frac{1}{2}J\langle f_{i\uparrow}^\dagger f_{i+\hat{x}\uparrow} \rangle$, $\tilde{t}' = xt'$. The expectation values $\langle \dots \rangle$ in \tilde{t} and $\Delta_0 = 2J \times [\langle f_{i\uparrow}^\dagger f_{i+\hat{x}\uparrow} \rangle - \langle f_{i\downarrow}^\dagger f_{i+\hat{x}\downarrow} \rangle]$ are computed self-consistently from minimization of the free energy. The hole concentration (doping) x sets the density of fermions $(1-x) = \sum_{\sigma} \langle f_{i\sigma}^\dagger f_{i\sigma} \rangle$ and bosons $\langle b_i \rangle = \sqrt{x}$.

The magnetic susceptibility is calculated in ladder approximation,

$$\chi(\mathbf{q}, \omega) = \chi^0(\mathbf{q}, \omega) / [1 + \alpha J(\mathbf{q}) \chi^0(\mathbf{q}, \omega)] \quad (1)$$

with $J(\mathbf{q}) = J[\cos(q_x) + \cos(q_y)]$ and $\alpha = 1$. Figure 1 shows $\chi^0(\mathbf{q}, \omega)$, which is built of fermion bubbles with a vertex function to include all ladder diagrams. Boson excitations do not appear in ladder approximation. Therefore the calculation does not distinguish between the SC and the spin-gap phase ($\Delta_0 \neq 0$ but $\langle b_i \rangle = 0$), and the persistence of the resonance above T_c in underdoped cuprates appears quite naturally.

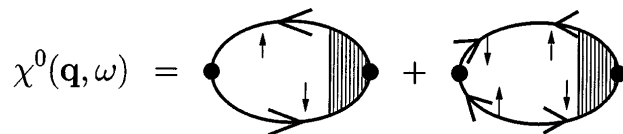


FIG. 1. Particle-hole irreducible contribution to the susceptibility Eq. (1). Single and double arrowed lines are normal and anomalous Green's functions of auxiliary fermions in the d -wave BCS state. Shaded areas denote the vertex function $\Lambda = 1 + \Lambda^J$. Λ^J accounts for all ladder diagrams not included in a simple random-phase approximation.

If $\chi(\mathbf{q}, \omega = 0)$ is computed from Eq. (1), an instability to an (incommensurate) Néel state occurs for hole densities $x < x_c \approx 0.2$. The high value of x_c is an artifact of the mean-field theory. Since the inclusion of fluctuations is beyond the scope of this work, we model the expected suppression [17,18] by setting $\alpha = 0.34$ in Eq. (1), such that x_c is reduced to an observed value 0.02. It is assumed that the superconducting phase $x > x_c$ is stable when fluctuations are included, at least for low T . A renormalization of the mean-field parameters, e.g., Δ_0 is ignored, in order to keep $\alpha \leftrightarrow x_c$ the only phenomenological input. The self-consistent $\Delta_0 \approx 45$ meV at optimal doping actually compares to experimental values [19]. We have checked numerically that the local moment sum rule is not sensitive to the choice of α .

With this approach we are able to access the full range of hole densities $0.02 < x < 0.15$ of underdoped cuprates. Numerical calculations are performed in the superconducting state at low temperature $T \rightarrow 0$ with parameters $t = 2J$, $t' = -0.45t$ for YBCO [20,21]. Figure 2 shows the imaginary part $\chi''(\mathbf{Q}_\pi, \omega)$ of Eq. (1) at the AF wave vector $\mathbf{Q}_\pi \equiv (\pi, \pi)$ for several hole concentrations. Apparently χ'' is dominated by a sharp resonance. For $x = 0.12$ it appears at an energy $\omega_0 = 0.51J \approx 60$ meV, its residual width is due to the small quasiparticle damping used in the numerical calculation. When doping is reduced to $x \approx 0.08 \rightarrow 0.04$ the resonance moves monotonously to lower energies and develops some damping. For further reduced hole filling, the peak becomes again resolution limited and eventually shifts to $\omega_0 \rightarrow 0$ when the AF tran-

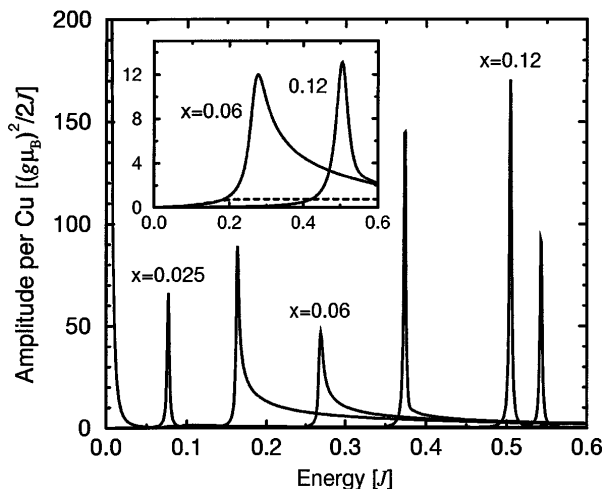


FIG. 2. Imaginary part χ'' of the susceptibility Eq. (1) for wave vector (π, π) . Main figure: Superconducting state at $T \rightarrow 0$; different peaks belong from left to right to hole concentrations $x = 0.02$ (scaled $\times 0.1$), 0.025 ($\times 0.1$), 0.04 , 0.06 , 0.08 , 0.12 , 0.16 . All peaks except $x = 0.04$, 0.06 , 0.08 are δ functions, computed with a quasiparticle damping $\Gamma = 10^{-3}J$. Inset: $x = 0.06$, 0.12 in the SC state (full lines) and $x = 0.12$ in the normal state $T \geq T_c$ (dashed line). Here an experimental energy resolution (FWHM) of 5 meV is simulated via $\Gamma = 0.01J$.

sition is reached at $x = x_c = 0.02$. The peak vanishes in the normal phase $T > T_c$ near optimal doping; see the inset of Fig. 2. In heavily overdoped systems $x > 0.2$ the resonance vanishes even in the SC state.

The qualitative agreement between these results and the experimental findings summarized in the beginning is quite satisfactory. The resonance position $\omega_0 \approx 60$ meV near optimal doping ($x = 0.12$) is not too far off the observed value 40 meV. We also calculated the AF correlation length ζ from the equal-time correlation function $\langle \mathbf{S}(\mathbf{q})\mathbf{S}(-\mathbf{q}) \rangle$. When doping is reduced, ζ increases monotonically and reaches the system size at $x = x_c = 0.02$. Quantitatively ζ is overestimated by a factor of ≈ 2 compared to known values [22,23].

It is at first sight surprising that the resonance occurs at energies $\omega_0 \lesssim 2\Delta_0$ without significant damping from particle-hole (p - h) excitations, since the d -wave SC phase has a finite density of states. Figure 3 shows the imaginary part $\chi^{0''}(\mathbf{Q}_\pi, \omega)$ of the p - h bubbles $\chi^0 = \chi^{0'} + i\chi^{0''}$ from Fig. 1, together with the real part of the denominator of Eq. (1), $K(\mathbf{Q}_\pi, \omega) = [1 + \alpha J(\mathbf{Q}_\pi)\chi^{0'}(\mathbf{Q}_\pi, \omega)]$. From the numerical calculation the vertex corrections have no effect on the outcome of Eq. (1) and are omitted here. $\chi^{0''}$ has a full gap up to an energy Ω_0 , which increases with doping. A pole occurs in Eq. (1) since the corresponding K crosses zero at an energy $\omega_0 < \Omega_0$ in the gap. The result is a δ -like resonance for a hole filling near the AF transition ($x = 0.025$) or near optimal doping ($x = 0.12$). In the underdoped case ($x = 0.06$) we have $\omega_0 \approx \Omega_0$, and the resonance is asymmetrically broadened. To explain this we note that apart from BCS

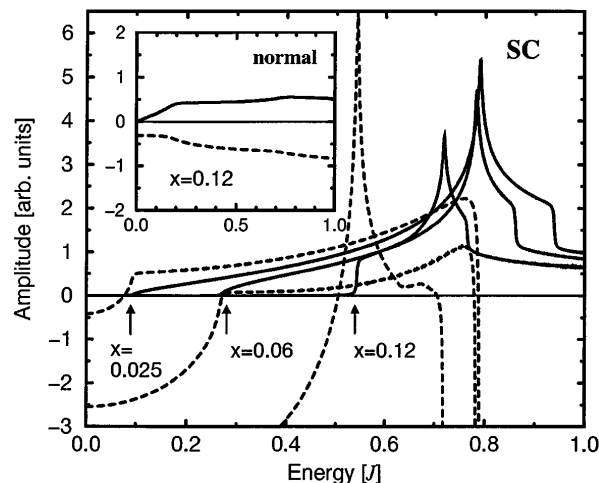


FIG. 3. Imaginary part $\chi^{0''}$ of the particle-hole bubbles from Fig. 1 for wave vector (π, π) (continuous lines), and the inverse Stoner enhancement factor K defined in the text [scaled $\times (-10)$, dashed lines]. Main figure: Shown are three hole fillings x in the SC state at $T \rightarrow 0$. An arrow points to the threshold energy Ω_0 in the respective $\chi^{0''}$; the corresponding K crosses zero at ω_0 nearby. $\chi^{0''}$ shows a van Hove singularity at $2\Delta_0 \approx 0.7J$ (a peak) and for $x = 0.12$ also at $\Omega_0 \approx 0.53J$ (a step). Inset: Normal state $T \geq T_c$ for $x = 0.12$.

coherence factors, $\chi^{00}(\mathbf{q}, \omega) \sim \sum_{\mathbf{k}} \delta[\omega - \Omega(\mathbf{q}, \mathbf{k})]$ at $T \rightarrow 0$, where $\Omega(\mathbf{q}, \mathbf{k}) = E(\mathbf{k}) + E(\mathbf{k} + \mathbf{q})$ and $E(\mathbf{k}) = \sqrt{\varepsilon^2(\mathbf{k}) + \Delta^2(\mathbf{k})}$. Here $\Omega(\mathbf{q}, \mathbf{k})$ denotes the p - h excitation energies of fermions with relative wave vector \mathbf{q} . For $\mathbf{q} = \mathbf{Q}_\pi$ this has a minimum value Ω_0 , which determines the threshold in χ^{00} . It is given by $\Omega_0 = 2|\mu_f|Z$, where μ_f is the fermion chemical potential and $Z = 1$ for $\kappa = \Delta_0^2/(4\mu_f\tilde{t}') > 2$ and $Z = \sqrt{\kappa - \kappa^2/4}$ for $0 < \kappa < 2$. Note that Ω_0 , and therefore the resonance energy ω_0 do not follow $2\Delta_0$.

The reason for the absence of damping at optimal doping ($x = 0.12$) is identified in the steplike Van Hove singularity (VHS) at $\omega = \Omega_0$ in χ^{00} (see Fig. 3), induced by a locally flat p - h dispersion. By virtue of the Kramers-Kronig transformation the real part $\chi^{0'}$ develops a sharp structure around Ω_0 , shifting the position ω_0 of the resonance (i.e., the zero crossing of K) well into the gap. When x is reduced, the VHS and with it the peak structure in $\chi^{0'}$ weaken, and ω_0 moves close to and may cross the threshold Ω_0 to damping p - h excitations. At very low doping $x \geq x_c$ this trend is over-compensated by the monotonous increase of χ^0 with reduced x , which shifts ω_0 back into the gap. The increase of χ^0 comes from the shrinking of the upper cutoff $2\tilde{W}$ for p - h excitations, with the bandwidth $\tilde{W} \approx 8\tilde{t} \approx 8(xt + J/8)$ of Gutzwiller renormalized fermions. It should be noted that the steplike VHS in χ^{00} near optimal doping depends on the coexistence of a finite Δ_0 and effective next-nearest-neighbor hopping \tilde{t}' , which lead to a sufficiently flat $\Omega(\mathbf{Q}_\pi, \mathbf{k})$. Setting $\tilde{t}' = 0$ eliminates the step, and the resonance from Eq. (1) is severely broadened. In the normal phase $\Delta_0 = 0$ no resonance appears at all. The p - h dispersion $\Omega(\mathbf{Q}_\pi, \mathbf{k}) = |\varepsilon(\mathbf{k})| + |\varepsilon(\mathbf{k} + \mathbf{Q}_\pi)|$ then has a zero minimum value without VHS, resulting in a gapless and structureless χ^{00} and K (see the inset of Fig. 3).

The approach presented here supports the understanding of the “41 meV resonance” as a collective spin fluctuation. We find that the sharp resonance is entirely caused by the pole in the random-phase approximation (RPA), which sums up spin-singlet particle-hole excitations, i.e., transversal spin fluctuations. The vertex function $\Lambda = 1 + \Lambda^J$ in χ^0 (see Fig. 1) has numerically no effect ($\Lambda^J \approx 0$) in the energy and doping range considered here. That is, we can neglect, in particular, the resonant contribution from spin-triplet particle-particle (p - p) pairs, which are involved through the mixing with p - h -excitations $f_{\mathbf{k}+\mathbf{Q}_\pi}^\dagger f_{\mathbf{k}\downarrow} \leftrightarrow f_{\mathbf{k}+\mathbf{Q}_\pi}^\dagger f_{-\mathbf{k}\uparrow}$ in the SC state [15]. Our view on the neutron scattering differs from, e.g., Ref. [15], where the p - p channel is considered the main contribution to the “41 meV resonance.” Some further comparison of these viewpoints has been given in Refs. [24,25].

We now turn to the discussion of the magnetic response in wave-vector space. The resonance at 41 meV, as well as its relative in underdoped samples at energies $\omega_0 < 41$ meV, is characterized as a single (commensurate)

peak at $\mathbf{q} = (\pi, \pi) = (1/2, 1/2)$ reciprocal-lattice units (r.l.u.) [3–5,7]. Recent INS experiments by Mook *et al.* [16], performed at an energy $\omega_i = 24$ meV $\approx 0.7\omega_0$ on an YBa₂Cu₃O_{6.6} sample with $\omega_0 = 34$ meV, gave evidence for an incommensurate response. It is dominated by four peaks, horizontally displaced from (π, π) . The maximum intensity is strongly reduced compared to $\omega = \omega_0$. Figure 4 shows $\chi''(\mathbf{q}, \omega)$ for $x = 0.12$ at $T \rightarrow 0$ from the renormalized RPA Eq. (1) with vertex corrections omitted. At the energy $\omega_0 = 0.51J$ (top panel) the susceptibility is commensurate [10]. When the energy is lowered to $\omega_i = 0.7\omega_0 = 0.3J$, the intensity drops dramatically, and four peaks appear at $\mathbf{q} = (\pi \pm \delta, \pi)$ and $(\pi, \pi \pm \delta)$, as is seen in the experiment [16]. The amount $\delta = 0.1$ r.l.u. of the displacement fits well the observed value 0.105 r.l.u. The incommensurate pattern may be characterized by the intensity ratio I_h/I_d , which is the maximum intensity I_h found in a horizontal scan through (π, π) , related to the maximum I_d from a diagonal scan. The numerical

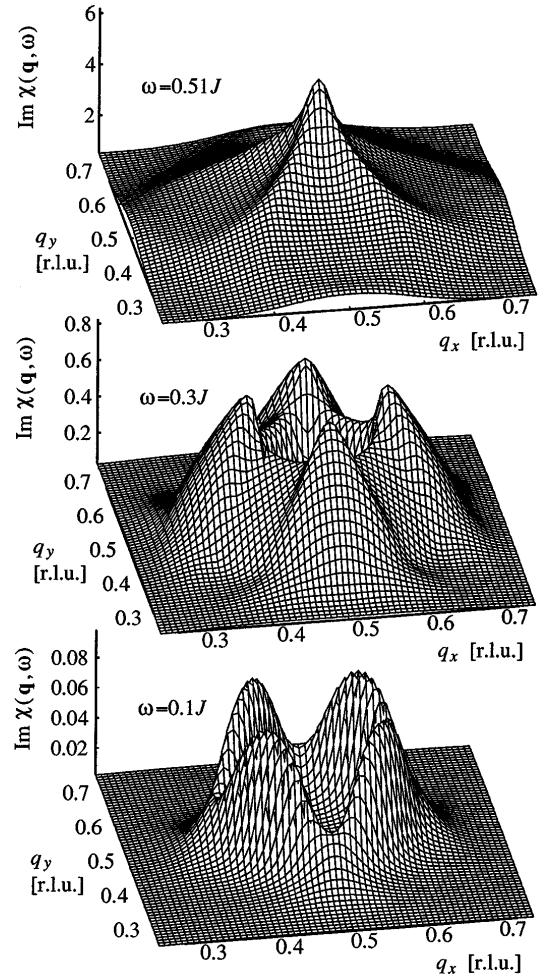


FIG. 4. Wave-vector scan of $\chi''(\mathbf{q}, \omega)$ (in arbitrary units) around $\mathbf{q} = (\pi, \pi)$ in the SC state at $T \rightarrow 0$. q_x, q_y are in units of $2\pi = 1$ r.l.u. The hole filling is $x = 0.12$, energies are $\omega = 0.51J = \omega_0$, $0.3J = 0.7\omega_0$, $0.1J$ (from top to bottom). A quasiparticle damping $\Gamma = 0.02J$ has been used.

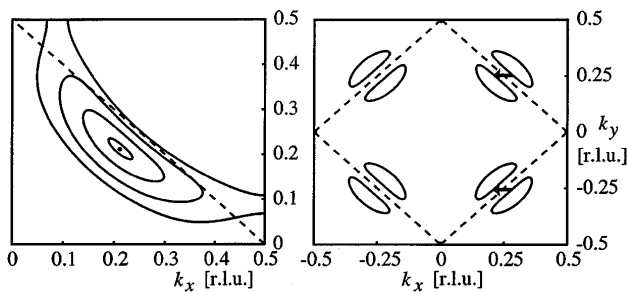


FIG. 5. Left: Contour plot of $E(\mathbf{k})$ in the SC state for $x = 0.12$. Shown is the upper right $1/4$ Brillouin zone (BZ) with $k_{x/y}$ in units of $2\pi = 1$ r.l.u. The node $E(\mathbf{k}) = 0$ appears as a dot, encircled by contours $E(\mathbf{k}) = \omega/2$ for $\omega = 0.1J$ (most inner curve), $0.3J$, $0.51J$, $0.7J$. Right: Contour for $\omega = 0.3J$ and its by (π, π) shifted image in the full BZ. Arrows indicate the best nesting vector relative to (π, π) .

calculation yields $I_h/I_d = 1.4$; from the data given in Ref. [16] we estimate an experimental value ≤ 2.0 . When the energy is further reduced, I_h/I_d changes continuously to values < 1 , and for $\omega \ll \omega_0$ (bottom panel) four peaks appear at $\mathbf{q} = (\pi \pm \delta', \pi \pm \delta')$ [9,26]. At these low energies no information on the \mathbf{q} -space structure has yet been obtained from INS, due to the very dim intensity.

An explanation for the incommensurate pattern at $\omega = \omega_i$ can be found in the quasiparticle dispersion $E(\mathbf{k})$ of the d -wave SC state. Consider again the p - h excitation energies $\Omega(\mathbf{q}, \mathbf{k})$. At low energy $\omega \rightarrow 0$ only excitations between the nodes $E(\mathbf{k}) \geq 0$, $E(\mathbf{k} + \mathbf{q}) \geq 0$ contribute, with $\mathbf{q} = (\pi \pm \delta', \pi \pm \delta')$ near (π, π) [26]. For small $\omega = 0.1J$ this is still the dominant process; see Fig. 5 (left). The situation changes for $\omega = \omega_i = 0.3J$. The contour $E(\mathbf{k}) = \omega_i/2$ contains a flat piece, which allows for a nesting contribution from (nearly) degenerate excitations $E(\mathbf{k}) \approx E(\mathbf{k} + \mathbf{q}) = \omega_i/2$. Following Ref. [27] the best nesting vector is a horizontal (or vertical) offset to (π, π) , i.e., $\mathbf{q} = (\pi \pm \delta, \pi)$ and $(\pi, \pi \pm \delta)$. This is illustrated in Fig. 5 (right); the offset is given by $\delta = \arcsin[(\omega + \mu_f)/\tilde{t}]$. The above reasoning has been given without consideration of the renormalized RPA, Eq. (1), since, in fact, $\chi \approx \chi^0$ for energies below ω_0 . On the other hand, this is not the case near the resonance energy $\omega_0 = 0.51J$, where χ is determined by a pole in Eq. (1), which produces the strong commensurate peak displayed in the top panel of Fig. 4.

In conclusion, we find that the slave-boson mean-field theory, enhanced by the renormalized RPA, gives a reasonable explanation for the INS experiments on $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ compounds. The energy and vanishing damping of the “41 meV resonance” is associated with the threshold of p - h excitations at $\mathbf{q} = (\pi, \pi)$. The evolution of the resonance with hole filling is accounted for, but

the damping is quite sensitive to the band structure (i.e., $t' \neq 0$). The same theory explains the incommensurate structure at lower energies as a dynamic nesting effect, specific to the d -wave SC state.

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