Energy Scales in the Local Magnetic Excitation Spectrum of YBa$_2$Cu$_3$O$_{6+y}$

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The wave-vector integrated dynamical spin susceptibility $\chi_{2D}(\omega)$ of YBa$_2$Cu$_3$O$_{6+y}$ cuprates is considered. $\chi_{2D}$ is calculated in the superconducting state from a renormalized mean-field theory of the $t$–$t'$–$J$-model, based on the slave-boson formulation. Besides the well-known “41 meV resonance” a second, much broader peak ('hump') appears in $\mathrm{Im}\chi_{2D}$. It is caused by particle–hole excitations across the maximum gap $\Delta_0$. In contrast to the resonance, which moves to lower energies when the hole filling is reduced from optimal doping, the position of this ‘hump’ at $\approx 2\Delta_0$ stays almost unchanged. The results are in reasonable agreement with inelastic neutron-scattering experiments.

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1. INTRODUCTION

The most prominent feature in the magnetic excitation spectrum of YBa$_2$Cu$_3$O$_{6+y}$ (YBCO) and Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO) cuprates is the so-called “41 meV resonance” at the antiferromagnetic (AF) wave vector $\mathbf{q} = (\pi, \pi)$. Its energy $\omega_{\text{res}}$ is $\approx 40$ meV in optimally doped samples and decreases with underdoping down to $\omega_{\text{res}} \approx 24$ meV. Recently the magnetic response has also been studied by averaging the neutron-scattering data over the in-plane 2D Brillouin zone. The resulting local magnetic excitation spectrum $\mathrm{Im}\chi_{2D}(\omega)$ shows the above-mentioned resonance and a second, hump-like feature at an energy $\omega_{\text{hump}}$ above $\omega_{\text{res}}$. In contrast to $\omega_{\text{res}}$, $\omega_{\text{hump}}$ depends only weakly on the doping level. Within the calculation
to be presented in the following the ‘hump’ is naturally explained by particle–hole (ph) excitations across the maximum d-wave gap $\Delta^0$. The energy $\omega_{\text{hump}} \sim 2\Delta^0$ comes out almost independent of doping. The resonance, on the other hand, emerges from a ph-bound state in the magnetic (spin-flip) channel and shows a strong doping dependence.

2. MODEL AND MEAN-FIELD THEORY

Our starting point is the doped Mott insulator. We study the $t$–$J$-model on a simple square lattice of Cu-3d orbitals for each of the two coupled CuO$_2$ layers (planes) in YBCO or BSCCO:

$$H = - \sum_{\nu,\nu',\sigma} t_{\nu\nu'} \tilde{c}^\dagger_{\nu\sigma} \tilde{c}_{\nu'\sigma} + \frac{1}{2} \sum_{\nu,\nu'} J_{\nu\nu'} \vec{S}_\nu \vec{S}_{\nu'} .$$

(1)

In the subspace with no doubly occupied orbitals, the electron operator on a Cu-lattice site $\nu$ is denoted $\tilde{c}_{\nu\sigma}$ with spin index $\sigma = \pm 1$; $\vec{S}_\nu$ is the spin-density operator. A Cu-site is specified through $\nu \equiv [i, l]$, where $i = 1 \ldots N_L$ indicates the Cu-position within one CuO$_2$-plane and $l = 1, 2$ selects the layer. $t_{\nu\nu'}$ denotes the effective intra- and inter-layer Cu–Cu-hopping matrix elements, and $J_{\nu\nu'}$ the antiferromagnetic super exchange. To deal with the constraint of no double occupancy, the standard auxiliary-particle formulation $\tilde{c}_{\nu\sigma} = b^\dagger_{\nu\sigma} f_{\nu\sigma}$ is used. The fermion $f^\dagger_{\nu\sigma}$ creates a singly occupied site (with spin $\sigma$), the “slave” boson $b^\dagger_{\nu\sigma}$ an empty one out of the (unphysical) vacuum $b_{\nu\sigma}|0\rangle = f_{\nu\sigma}|0\rangle = 0$. The constraint now takes the form $Q_\nu = b^\dagger_{\nu\sigma} b_{\nu\sigma} + \sum_\sigma f^\dagger_{\nu\sigma} f_{\nu\sigma} = 1$. In mean-field theory the constraint is relaxed to its thermal average $\langle Q_\nu \rangle = 1$. Together with the number $x$ of doped holes per Cu-site, it fixes the fermion and boson densities to

$$\langle 1 - x \rangle = \sum_\sigma \langle f^\dagger_{\nu\sigma} f_{\nu\sigma} \rangle , \quad \langle x \rangle = \langle b^\dagger_{\nu\sigma} b_{\nu\sigma} \rangle .$$

(2)

The derivation of mean-field equations is presented in Ref. 12. The dynamical spin susceptibility is given in units of $(g\mu_B)^2$ as

$$\chi(q, q_z, \omega) = \chi^+(q, \omega) \cos^2 \left( \frac{d}{2} q_z \right) + \chi^-(q, \omega) \sin^2 \left( \frac{d}{2} q_z \right) ,$$

where $q$ is the in-plane wave vector, $d$ denotes the distance of CuO$_2$ planes within a double-layer sandwich. For the even (+) and odd (−) mode susceptibilities a RPA-type expression is obtained,

$$\chi^\pm(q, \omega) = \frac{\chi^{\text{ irr}}_{\pm}(\omega)}{1 + J^\pm(q) \chi^{\text{ irr}}_{\pm}(\omega)} .$$

(3)
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The irreducible part $\chi^{\text{irr}}$ consists of a particle–hole (ph) bubble of fermions as is known from BCS theory,

$$\chi^{\text{irr}}_p(\omega) = \frac{1}{2N_L} \sum_{\mathbf{k},\mathbf{p}_z} \sum_{s,s'=\pm 1} \frac{1}{8} \left[ 1 + s s' \omega \Delta' \frac{f(s'E') - f(sE)}{\omega + sE - s'E' + i\delta} \right]$$

with $p \equiv (\mathbf{q}, p_z)$ and $p_z = \{0, \pi\}$ for the modes $\{+, -\}$. Boson excitations do not enter $\chi$ on mean-field level. Fermions obey an effective dispersion $\varepsilon \equiv \varepsilon(\mathbf{k}, \mathbf{p}_z), \varepsilon' \equiv \varepsilon(\mathbf{k} + \mathbf{q}, \mathbf{p}_z + p_z),$

$$\varepsilon(\mathbf{k}, \mathbf{p}_z) = -2\tilde{t}[\cos(k_x) + \cos(k_y)] - 4\tilde{t}' \cos(k_x) \cos(k_y) - \tilde{t}^\perp(\mathbf{k}) e^{i\tilde{p}_z}$$

and d-wave gap function $\Delta \equiv \Delta(\mathbf{k}, \mathbf{p}_z), \Delta' \equiv \Delta(\mathbf{k} + \mathbf{q}, \mathbf{p}_z + p_z),$

$$\Delta(\mathbf{k}, \mathbf{p}_z) = \frac{\Delta_0}{2} \left[ \cos(k_x) - \cos(k_y) \right] + \Delta_0^1 e^{i\tilde{p}_z}$$

These enter the usual quasi-particle energy $E = \sqrt{\varepsilon^2 + \Delta^2}, E' = \sqrt{\varepsilon'^2 + \Delta'^2}$. Formally, vertex corrections to the simple bubble Eq. (4) have to be taken into account. However, these have almost no effect in the energy-range below $2\Delta^0$ and are therefore ignored in the following.

From Feynman’s variation principle the effective hopping parameters are determined as $\tilde{t} \approx xt + 0.15J, \tilde{t}' = xt', \tilde{t}^\perp(\mathbf{k}) \approx xt^\perp(\mathbf{k})$. For the bare nearest and next-nearest neighbor hopping we assume $t = 2J, t' = -0.45t, \text{and for the inter-plane hopping} \tilde{t}^\perp(\mathbf{k}) = 2t^\perp[\cos(k_x) - \cos(k_y)]^2 + t_0^\perp$ with $t^\perp = 0.1t$ and $t_0^\perp = 0$. We assume an in-plane superconducting order parameter $\Delta_0$ with equal amplitude and phase in both layers. The self-consistent solution of the mean-field equations then leads to a vanishing inter-plane gap $\Delta_0^\perp = 0$.

Magnetic excitations in the superconducting phase are described by quasi particles (the fermions) in a BCS-type d-wave pairing state. These propagate with effective hopping parameters $\tilde{t}, \tilde{t}'$ strongly reduced from the bare parameters $t, t'$ by the small Gutzwiller factor $x$. The bubble Eq. (4) describes spin-flip ph-excitations of these particles, which are subject to the mode-dependent final-state interaction in Eq. (5).

$$\tilde{J}^\pm(\mathbf{q}) = \alpha J(\mathbf{q}) \pm J^\perp, \quad J(\mathbf{q}) = 2J[\cos(q_x) + \cos(q_y)]$$

The inter-plane exchange is chosen as $J^\perp = 0.2J$. The destruction of the antiferromagnetic (AF) state of the $1/2$-filled system by hole doping is missing in mean-field theory. The necessary correlations of fermions and bosons are not contained, and the AF order vanishes at an unphysically high doping level $x'^0 \approx 0.22$. Therefore we assume a renormalization
$J \to \alpha J$ of the in-plane nearest-neighbor exchange. Using $\alpha = 0.35$ reduces $x_0^0$ down to $x_c \approx 0.03$, which is consistent with experiment and makes the study of underdoped systems possible. Note that the above-mentioned renormalization $t \to \tilde{t}$ of the quasi-particles comes out of the self-consistent calculation, whereas $J \to \alpha J$ is a phenomenological model. Our assumption of $\alpha$ being independent of doping leads to an AF correlation length $\xi_{AF}(x) \sim 1/\sqrt{x-x_c}$ at $T \to 0$, which agrees with known experimental and theoretical results.

3. RESULTS

From the susceptibility Eq. (3) the local magnetic excitation spectrum is determined from

$$\text{Im} \chi_{\pm 2D}(\omega) = \int_{-\pi}^{\pi} \frac{d^2q}{(2\pi)^2} \text{Im} \chi_{\pm}(q, \omega)$$

Fig. 1 shows $\text{Im} \chi_{2D}$ for the odd and even mode at $T \to 0$ in the superconducting state. A resonance is clearly visible in the odd ($-$) mode, at an energy $\omega_{\text{res}} \approx 0.42 J \approx 50 \text{ meV}$ for $x = 0.12$ near optimal doping. When $x$ is reduced (underdoping) the resonance moves to lower energies and gains spectral weight. The resonance appears at the same energy as in $\text{Im} \chi_{\pm}(q, \omega)$ for fixed wave vector $q = (\pi, \pi)$. In addition, both modes $\text{Im} \chi_{\pm 2D}(\omega)$ show a broad peak ('hump') at energies $\omega_{\text{hump}}^\pm \approx \omega_{\text{hump}}^\pm$ above $\omega_{\text{res}}$. In contrast to $\omega_{\text{res}}$ the hump-maxima $\omega_{\text{hump}}^\pm$ are almost independent of doping, located somewhat below $2\Delta^0$ ($2\Delta^0 \approx 0.7 J$ for $x = 0.12$).

The resonance emerges from a pole in Eq. (5) at wave-vector $(\pi, \pi)$ and energy $\omega_{\text{res}}$, driven by the effective interaction Eq. (5) in the odd ($-$) mode. Since $\omega_{\text{res}}$ is slightly below the threshold $\Omega_0$ to the particle–hole (ph) continuum, the resonance appears undamped, i.e., as a $\delta$-function. Due to the inter-layer coupling $J^\perp$ the interaction Eq. (5) is weaker in the even (+) mode, and the resonance in $\text{Im} \chi_{\pm}$ is shifted up into the ph-continuum, becoming almost suppressed. Consequently, in wave-vector space a sharp peak around $(\pi, \pi)$ is visible only in the odd ($-$) mode. This is demonstrated in the top panel of Fig. 2. The bottom panel of that figure shows the magnetic response at a higher energy close to the hump-maxima $\omega_{\text{hump}}^\pm$. The intensity is much reduced compared to the resonance. However, the magnetic excitations at $\approx \omega_{\text{hump}}$ occupy almost the whole 2D Brillouin zone, and despite their small amplitude they contribute to the wave vector integrated susceptibility Eq. (6). The ‘hump’ can be traced back to ph-exitations across the maximum gap $\Delta^0$: At $q = (\pi, \pi)$ the irreducible particle–hole
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Fig. 1. Wave-vector $q$ integrated odd- and even-mode susceptibilities $\text{Im}\chi^{(2D)}$ for hole filling $x = 0.06 \ldots 0.18$. Parameters are $t = 2J$, $t' = -0.45t$, $t^\perp = 0.1t$, $J^\perp = 0.2J$. Curves are calculated with a damping FWHM = 0.04$J \approx 5$ meV. Inset: $q$-integrated bubble spectrum $\text{Im}\chi^{(2D)}_{\text{irr}}$ for $x = 0.08$. The maximum is located close to $2\Delta^0 = 0.78J$. 

bubble $\text{Im}\chi^{\text{irr}}(q, \omega)$ shows a log-type van Hove singularity (vHs) at $\omega = 2\Delta^0$, remnant of the density of states of the d-wave superconductor. Moving off ($\pi, \pi$) this vHs splits into three vHs that disperse very weakly throughout the Brillouin zone, leading to a soft maximum ('hump') at $2\Delta^0$ in the $q$-integrated (local) bubble spectrum $\text{Im}\chi^{(2D)}_{\text{irr}}(\omega)$. This is shown in the inset of Fig. 1. When the final-state interaction Eq. (3) is taken into account, the resonance is obtained in the odd mode, and the hump is pulled down to $\omega^-_{\text{hump}} < \omega^+_{\text{hump}} < 2\Delta^0$. Also is the doping dependence of $\Delta^0$ compensated: $\omega^\pm_{\text{hump}}$ are independent of doping, while $\Delta^0$ increases with underdoping.
Fig. 2. Magnetic response $\text{Im}\chi^{(\pm)}$ (in arbitrary units) in wave-vector $\mathbf{q}$ space for $x = 0.08$. $q_x$, $q_y$ are measured in units of $2\pi = 1\text{r.l.u.}$ Parameters as in Fig. 1. Top: At the energy $\omega = \omega_{\text{res}}$ where the resonance appears in the odd mode. Bottom: At an energy $\omega$ close to the ‘hump’-maxima in both modes. (Note the different amplitude scale.)

4. COMPARISON TO EXPERIMENT

Two experimental groups studied the wave-vector integrated magnetic response $\text{Im}\chi^{(\pm)}_{2D}$ in underdoped YBCO. Refs. [1][2] reported a line shape for YBCO$_{6.6}$, which agrees quite well with our theoretical result for $x \leq 0.08$. A ‘hump’ in $\text{Im}\chi^{+}_{2D}$ (even) appears at $\approx 100\text{meV}$, $\text{Im}\chi^{-}_{2D}$ (odd) shows a similar structure at a somewhat lower energy $\approx 90\text{meV}$. The well-known resonance appears only in $\text{Im}\chi^{-}_{2D}$ at 34 meV. In Refs. [3][4] two underdoped samples YBCO$_{6.7}$ and YBCO$_{6.5}$ have been studied. In the even (“optical”) mode of YBCO$_{6.7}$ a hump appears around 70 meV, whereas the odd (“acoustic”)
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mode shows a weak hump-like structure at $\approx 55$ meV, separated from the resonance at 33 meV. These features tend to move up in energy in the more underdoped sample YBCO$_{6.5}$, while the resonance in $\text{Im} \chi_{2D}^\pm$ shifts down to 25 meV.

Although the detailed experimental line shapes are not unique, the qualitative features of our calculation are found in the neutron-scattering spectra. In particular we reproduce the different dependencies on doping level of the resonance at $\omega_{\text{res}}$ in the odd mode and the hump-like feature at $\omega_{\text{hump}}^\pm$ in both modes. Also is $\omega_{\text{hump}}^-$ of the odd mode lower than the $\omega_{\text{hump}}^+$ of the even mode. Theory and experiments can also be compared quantitatively.

The measured neutron-scattering intensities are of the same order as the theoretical ones in Fig. 1 (using $J =$ 120 meV, i.e., $1\mu_B^2/J = 8.3\mu_B^2/eV$). The maximum of the hump in the even, odd mode in Fig. 1 occurs at $\omega^{+,-} \approx 0.53J = 72$ meV, 64 meV, in good agreement with the measurements Ref. 9 on YBCO$_{6.7}$ at low temperature.

![Graph](image.png)

Fig. 3. $2|\mu^f|$, $2\Delta^0$, the ph-threshold $\Omega_0$, and the resonance energy $\omega_{\text{res}}$ as function of doping at $T \to 0$.

5. CONCLUSION

The local magnetic excitation spectrum $\text{Im} \chi_{2D}^\pm(\omega)$ is characterized by two energy scales that behave differently with hole filling $x$ (doping). The
resonance energy $\omega_{\text{res}}$ follows the particle–hole threshold $\Omega_0$, which in underdoped systems is determined by the chemical potential $\mu_f$ of the fermions as $\omega_{\text{res}} \leq \Omega_0 = 2|\mu_f|$. The maxima of the humps, on the other hand, are determined by the gap $\Delta^0$ through $\omega_{\text{hump}}^\pm \sim 2\Delta^0$. When $x$ is reduced from optimal doping, $|\mu_f|$ and therefore $\omega_{\text{res}}$ decrease quickly, while $\Delta^0$ increases. This is displayed in Fig. 3. It has been noted above that the mean-field theory describes magnetic excitations in terms of quasi particles (QP) (the fermions) with a reduced Fermi velocity $\bar{v}_F \approx (x + 0.15J/t)v_F$. Hence in underdoped systems the QP’s chemical potential comes out (much) smaller than the gap, $|\mu_f| < \Delta^0$, and thus determines the scale for $\omega_{\text{res}}$. This leads to the observed decoupling of the resonance energy from the gap $\Delta^0$, while $\Delta^0$ is still visible through the ‘humps’ in the local spectrum $\text{Im} \chi_{2D}$.

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