Journal of Magnetism and Magnetic Materials 374 (2015) 624–633

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Dynamical spin response in cuprate superconductors from low-energy to high-energy

Lülin Kuang [a], Yu Lan [b], Shiping Feng [a,*]

[a] Department of Physics, Beijing Normal University, Beijing 100875, China
[b] Department of Physics and Electronic Information Science, Hengyang Normal University, Hengyang 421002, China

ARTICLE INFO

Article history:
Received 30 July 2014
Available online 16 September 2014

Keywords:
Dynamical spin response
Commensurate resonance
Cuprate superconductor

ABSTRACT

Within the framework of the kinetic energy driven superconducting mechanism, the dynamical spin response of cuprate superconductors is studied from low-energy to high-energy. The spin self-energy is evaluated explicitly in terms of the collective charge carrier modes in the particle–hole and particle–particle channels, and employed to calculate the dynamical spin structure factor. Our results show the existence of damped but well-defined dispersive spin excitations in the whole doping phase diagram. In particular, the low-energy spin excitations in the superconducting-state have an hour-glass-shaped dispersion, with commensurate resonance that appears in the superconducting-state *only*, while the low-energy incommensurate spin fluctuations can persist into the normal-state. The high-energy spin excitations in the superconducting-state on the other hand retain roughly constant energy as a function of doping, with spectral weights and dispersion relations comparable to those in the corresponding normal-state. The theory also shows that the unusual magnetic correlations in cuprate superconductors can be ascribed purely to the spin self-energy effects which arise directly from the charge carrier–spin interaction in the kinetic energy of the system.

1. Introduction

The interplay between antiferromagnetism and superconductivity is one of the challenging issues in cuprate superconductors [1–3]. This follows from a fact that the parent compounds of cuprate superconductors are a form of nonconductor called a Mott insulator with an antiferromagnetic (AF) long-range order (AFLRO) [2,3], where a single common structural feature is the presence of the CuO_2 planes. Furthermore, the inelastic neutron scattering (INS) experiments have shown that the low-energy spin excitations in these parent compounds are well described by an AF Heisenberg model [2–6] with magnetic exchange coupling constant $J \sim 0.1$ eV. The spin excitations with AFLRO are called as magnons. When the CuO_2 planes are doped with charge carriers, the AFLRO phase subsides and superconductivity emerges leaving the AF short-range order (AFSRO) correlations still intact. This AFSRO can still support spin waves, but the spin excitations with AFSRO are damped. The damped spin excitations are known as paramagnons [7]. In particular, in the doped regime, the charge carriers couple to the spin excitations [8,9], and it has been argued that if the spin excitations exist over a wide enough range of energies, they can produce the necessary attractive interaction to induce superconductivity [7–9].

The early INS measurements [3,8–16] on cuprate superconductors have demonstrated that the doped charge carriers cause substantial changes to the low-energy spin excitation spectrum, and a consistent pattern has been identified as the *hour-glass-shaped* dispersion. This hour-glass-shaped dispersion was first observed in the spin excitations of $YBa_2Cu_3O_{6.6}$ [15] and $La_{1.875}Ba_{0.125}CuO_4$ [16], where two incommensurate (IC) components of the low-energy spin excitation spectrum are separated by a commensurate resonance energy ω_r at the waist of the hour glass. In the upward component, above the commensurate resonance energy ω_r, the spin excitation spectrum is similar to what one would expect from AF spin fluctuations with a finite gap, and it is relevant to the results for different families of cuprate superconductors that appear to scale with the magnetic exchange coupling constant J for the parent Mott insulators. Moreover, for a given excitation energy, the magnetic scattering peaks lie on a circle of radius of $\overline{\delta}_{IC}'$, with the incommensurability parameter $\overline{\delta}_{IC}'$ that is defined as a deviation of the peak position from the AF wave vector $[1/2, 1/2]$ (hereafter we use the units of $[2\pi, 2\pi]$) in the Brillouin zone (BZ), and then the distribution of the spectral weight of the IC magnetic scattering peaks is rather isotropic. On the other hand, in the downward component, below ω_r, the distribution of the spectral weight of the IC magnetic scattering peaks is quite anisotropic [3,8–16]. In particular, it is remarkable [3,8–21] that in analogy to the domelike shape of the

* Corresponding author. Tel.: +86 10 58806408; fax: +86 10 58801764.
E-mail address: spfeng@bnu.edu.cn (S. Feng).

http://dx.doi.org/10.1016/j.jmmm.2014.09.018
0304-8853/

doping dependence of the SC transition temperature T_c, the commensurate resonance energy ω_r increases with increasing doping in the underdoped regime, and reaches a maximum around the optimal doping, then decreases in the overdoped regime, reflecting a intrinsical relationship between ω_r and T_c. Although the IC magnetic scattering has been also observed in the normal-state, the commensurate resonance is a new feature that appears in the SC-state *only* [3,8–21]. Later, this hour-glass-shaped dispersion was found in several different families of cuprate superconductors [22–25]. However, because of technical limitations, only the low-energy ($E \sim 10-80$ meV) spin excitations in a small range of momentum space around the AF wave vector are detected by the INS measurements [8–25], and they may be insufficient to produce superconductivity [7,8,26]. In recent years, instrumentation for resonant inelastic X-ray scattering (RIXS) with both soft and hard X-rays has improved dramatically, allowing this technique to directly measure the high-energy($E \sim 80$–500 meV) spin excitations of cuprate superconductors in the wide energy–momentum window that cannot be detected by the INS measurements [27]. In this case, as a compensation for the miss of a significant part of the spectral weight of the spin excitations in the INS studies [8–25], the RIXS experiments [27–31] have purported to measure high-energy spin excitations in a large family of cuprate superconductors that persist well into the overdoped regime and bear a striking resemblance to those found in the parent compound [32–34], indicating that a local-moment picture accounts for the observed spin excitations at elevated energies even up to the overdoped regime. In particular, the very importance is that the combination of these RIXS-INS experimental data have identified the spin excitations with high intensity over a large part of moment space, and shown that the spin excitations exist across the entire range of the SC dome, and with sufficient intensity to mediate superconductivity in cuprate superconductors [7,8,26].

Although the spin excitation spectrum of cuprate superconductors from low-energy to high-energy in the whole doping phase diagram is well-established from the INS [3,8–25] and RIXS [27–31] measurements, its full understanding is still a challenging issue. In our early studies [35,36], the low-energy spin excitations of the underdoped cuprate superconductors in the normal-state have been discussed by considering spin fluctuations around the mean-field (MF) solution, where the spin self-energy is evaluated from the charge carrier bubble in the particle–hole channel, and then the obtained results are qualitatively consistent with the corresponding experimental data. In this paper, as a complement of our previous analysis of the low-energy spin excitations of the underdoped cuprate superconductors in the normal-state, we start from the kinetic energy driven SC mechanism [37–39] to discuss the dynamical spin response of cuprate superconductors from low-energy to high-energy in both the SC- and normal-states, where one of our main results is that both damped but well-defined dispersive low-energy and high-energy spin excitations exist across the whole doping phase diagram. The low-energy spin excitations are strongly renormalized due to the charge carrier–spin interaction to form an hour-glass-shaped dispersion in the SC-state. In particular, we identify that the commensurate resonance is closely related to the process of the creation of charge carrier pairs, and appears in the SC-state only, while the low-energy IC magnetic scattering is mainly associated with the motion of charge carrier quasiparticles, and therefore can persist into the normal-state. On the other hand, the charge carrier doping has a more modest effect on the high-energy spin excitations, and then the high-energy spin fluctuations bear a striking resemblance to those found in the parent compound.

The paper is organized as follows. The basic formalism is presented in Section 2, where we evaluate explicitly the full spin Green's function (then the spin self-energy) in the SC-state in terms of the collective charge carrier modes in the particle–hole and particle–particle channels. The dynamical spin structure factor, however, is obtained from the imaginary part of the full spin Green's function, and is employed to discuss the quantitative characteristics of the dynamical spin response in cuprate superconductors in Section 3 for the SC-state and Section 4 for the normal-state, where we show that although the magnetic scattering of spins dominates the spin dynamics, the effect of charge carriers on the spin part in terms of the spin self-energy renormalization is critical in determining the doping and energy dependence of the dynamical spin response in cuprate superconductors.

2. Dynamical spin response in cuprate superconductors

Since the single common element in cuprate superconductors is the presence of the CuO_2 planes as mentioned above, it is believed that the anomalous properties are closely related to the doped CuO_2 planes [1,40,41]. In particular, as originally emphasized by Anderson [1], the essential physics of the doped CuO_2 plane is properly captured by the *t-J* model on a square lattice,

$$H = -t\sum_{l\hat{\eta}\sigma} C^{\dagger}_{l\sigma}C_{l+\hat{\eta}\sigma} + t'\sum_{l\hat{\tau}\sigma} C^{\dagger}_{l\sigma}C_{l+\hat{\tau}\sigma} + \mu\sum_{l\sigma} C^{\dagger}_{l\sigma}C_{l\sigma} + J\sum_{l\hat{\eta}} \mathbf{S}_l \cdot \mathbf{S}_{l+\hat{\eta}}, \quad (1)$$

where the summation is over all sites l, and for each l, over its nearest-neighbors $\hat{\eta}$ or the next nearest-neighbors $\hat{\tau}$, $C^{\dagger}_{l\sigma}$ ($C_{l\sigma}$) is the electron creation (annihilation) operator, $\mathbf{S}_l = (S^x_l, S^y_l, S^z_l)$ are spin operators, t (t') is the nearest-neighbor (next nearest-neighbor) hopping integral, J is the AF exchange coupling constant, and μ is the chemical potential. In this *t-J* model (1), the kinetic energy term describes the motion of charge carriers, while the Heisenberg term describes the AF coupling between localized spins. In particular, the nearest-neighbor hopping integral t in the kinetic energy term is much larger than the AF exchange coupling constant J in the Heisenberg term, and then the AF spin configuration is strongly affected by the motion of charge carriers. The high complexity in the *t-J* model comes mainly from the local constraint of no double electron occupancy, i.e., $\sum_{\sigma} C^{\dagger}_{l\sigma}C_{l\sigma} \le 1$, which can be treated properly within the charge–spin separation (CSS) fermion-spin theory [36,39,42], where the constrained electron operators $C_{l\uparrow}$ and $C_{l\downarrow}$ are decoupled as

$$C_{l\uparrow} = h^{\dagger}_{l\uparrow}S^{-}_l, \quad C_{l\downarrow} = h^{\dagger}_{l\downarrow}S^{+}_l, \quad (2)$$

respectively, with the fermion operator $h_{l\sigma} = e^{-i\Phi_{l\sigma}}h_l$ that keeps track of the charge degree of freedom together with some effects of spin configuration rearrangements due to the presence of the doped hole itself (charge carrier), while the spin operator S_l represents the spin degree of freedom, and then the local constraint of no double electron occupancy is always satisfied in analytical calculations. In this CSS fermion-spin representation (2), the original *t-J* model (1) can be expressed explicitly as

$$\begin{aligned} H = {} & t\sum_{l\hat{\eta}} (h^{\dagger}_{l+\hat{\eta}\uparrow}h_{l\uparrow}S^{+}_l S^{-}_{l+\hat{\eta}} + h^{\dagger}_{l+\hat{\eta}\downarrow}h_{l\downarrow}S^{-}_l S^{+}_{l+\hat{\eta}}) \\ & - t'\sum_{l\hat{\tau}} (h^{\dagger}_{l+\hat{\tau}\uparrow}h_{l\uparrow}S^{+}_l S^{-}_{l+\hat{\tau}} + h^{\dagger}_{l+\hat{\tau}\downarrow}h_{l\downarrow}S^{-}_l S^{+}_{l+\hat{\tau}}) \\ & - \mu\sum_{l\sigma} h^{\dagger}_{l\sigma}h_{l\sigma} + J_{\rm eff}\sum_{l\hat{\eta}} \mathbf{S}_l \cdot \mathbf{S}_{l+\hat{\eta}}, \end{aligned} \quad (3)$$

where $S^{-}_l = S^x_l - iS^y_l$ and $S^{+}_l = S^x_l + iS^y_l$ are the spin-lowering and spin-raising operators for the spin $S = 1/2$, respectively, $J_{\rm eff} = (1-\delta)^2 J$, and $\delta = \langle h^{\dagger}_{l\sigma}h_{l\sigma}\rangle = \langle h^{\dagger}_l h_l\rangle$ is the charge carrier doping concentration. As a consequence, the kinetic energy in the *t-J* model (3) has been released as the charge carrier–spin interaction, which reflects that even the kinetic energy in the *t-J* model (1) has strong Coulombic contribution due to the restriction of no double