Resonance, Fermi surface topology, and Superconductivity in Cuprates

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The resonance, a collective boson mode, was usually thought to be a possible glue of superconductivity. We argue that it is rather a natural product of the $d$-wave pairing and the Fermi surface topology. A universal scaling $E_{res}/2\Delta_H^H \sim 1.0$ ($\Delta_H^H$ the magnitude of superconducting gap at hot spot) is proposed for cuprates, irrespective of the hole-/electron-doping, low-/high-energy resonance, monotonic/nonmonotonic $d$-wave paring, and the parameters selected. We reveal that there may exist two resonance peaks in the electron-doped cuprates. The low- and high-energy resonance, originated from the contributions of the different intra-band component, is intimately associated with the Fermi surface topology. By analyzing the data of inelastic neutron scattering, we conclude the nonmonotonic $d$-wave superconducting pairing symmetry in the electron-doped cuprates, which is still an open question.

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High-temperature superconductivity, arising from the charge carrier doping into their parent compounds, is one of the most challenging topics in condense matter physics[1]. The fundamental issue is what the glue of pairing is in cuprates. The superconductivity is generally believed to associate with some collective boson modes. For example, due to the proximity of antiferromagnetism and superconductivity, the spin fluctuations is often proposed to be the glue of pairing in the cuprates[2]. Understanding the nature of the spin fluctuation and its relation to the superconductivity are essential for the mechanism of High-$T_c$ cuprates. The inelastic neutron scattering(INS) provides a direct way to investigate the spin dynamics.

So far, the extensive INS experiments had been performed on cuprates[1, 3]. The significant differences of magnetic excitations had been found, i.e., the ‘hourglass’ and low-energy commensurate dispersion of magnetic excitation in hole- and electron-doped cuprates. However, a universal feature in the superconducting (SC) state is proposed. The resonance[4-11], a spin-triplet collective mode at $Q = (\pi, \pi)$, is discovered in both type of cuprates. The resonance energy $E_{res}$ is about 9.5meV, and 11meV, in the optimal doping NCCO[7], and PLCCO[8], respectively. This value is much enhanced in the hole-doped cuprates, e.g., 18meV in optimal doped LSCO, 47meV in TI2212, 56meV in Hg1201, etc (Detailed experimental data, see Ref.[10]). It is proposed that the ratio of $E_{res}/k_BT_c$ is fixed with the value about 5.8[7, 8]. However, Yu et al. argued that the universal scaling is $E_{res}/2\Delta_S^{AN} \sim 0.64$ ($\Delta_S^{AN}$ the SC gap at antinode) instead[10], which is also supported by the scanning tunnelling microscopy measurements[12]. Furthermore, the single resonance may be constituted by two separated sub-peaks in optimal doped NCCO[11], which seems to conflict with the above mentioned universal ratio. Nevertheless, the resonance is intimately related to the superconductivity. In this sense, the resonance is the essence of the superconductivity and possibly the candidate of the glue of superconductivity.

Based on the kinetic energy driven SC mechanism, a dome shaped doping dependent resonance energy is proposed in electron-doped cuprates. However, the intensity at given energy in the SC state is almost three orders of magnitude larger than that of the normal state[13]. Ismer et al. showed that the resonance can be regarded as an overdamped collective mode located near the particle-hole continuum[14]. Their results indicated that the resonance energy is sensitive to the parameters selected. Furthermore, those theories based on the single band description[15, 16] could not be able to take account of the properties of spin dynamics, for example, the commensurate magnetic excitation in electron-doped cuprates, as we argued in the previous paper[17]. To our knowledge, the possible linear scaling of resonance and its intrinsic relation to superconductivity have not been well established.

In this paper, the resonance is studied in details in the cuprates. The resonance energy linearly depends on the SC gap. A low-energy resonance emerges when the the hole-pocket develops in the electron-doped cuprates. The main features of the magnetic excitations are qualitatively consistent with the INS measurements. The resonance, coming from respective intra-band component, is dominated by the scattering between two hot spots. We argue that the resonance is a natural product of the $d$-wave pairing symmetry and Fermi surface topology rather than the glue of superconductivity. A universal scaling $E_{res}/2\Delta_S^H \sim 1.0$ with $\Delta_S^H$ the magnitude of superconducting gap at the hot spot, which is insen-
sitive to the selected details, is proposed instead of the experimentally suggested $E_{\text{res}}/2\Delta_{S}^{N} \sim 0.64$. We conclude that the SC pairing symmetry in electron-doped cuprates is the nonmonotonic $d$-wave. This manifests that the INS measurement can not only be used to judge the pairing symmetry, but also provides the details.

We start from the generic model with non-zero Q-commensurate density wave, which assumes a $Q = (\pi, \pi)$ vector with an energy gap $\Delta_{k}^{N}$ that either is isotropic or has $d$-wave symmetry[18]. The Green’s function is

$$G_{k}^{-1} = \omega - \epsilon_{k} + i\Gamma - \frac{(\Delta_{k}^{N})^{2}}{\omega - \epsilon_{k} + Q + i\Gamma} \quad (1)$$

with $\epsilon_{k}$ the dressed tight-binding (TB) dispersion and $\Gamma$ the elastic broadening factor. This nonzero Q scenario, originated from the spin density wave[19], charge density wave[20], d-density-wave (DDW)[21], or spin-singlet correlations (SSC)[22] etc., well models the normal state surface topology in the underdoped cuprates. In the superconducting state, we introduce a phenomenological pairing term $-\sum_{k} \Delta_{k}^{S}(c_{k+Q}^\dagger c_{k} + h.c.)$, where $\Delta_{k}^{S} = \frac{1}{2}\Delta_{S}^{\pm}\xi(\cos k_{x} - \cos k_{y})$ is the monotonic d-wave SC order parameter usually. However, a nonmonotonic $d$-wave with high harmonic term[23, 24] $\Delta_{k}^{S} = \frac{1}{2}\Delta_{S}^{\pm}\xi(\cos k_{x} - \cos k_{y}) - \Delta_{k}^{2} N(\cos 3k_{x} - \cos 3k_{y})$ is further discussed in the electron-doped case with $\Delta_{S}^{\pm} \sim \Delta_{S}/2.41[16]$. The quasiparticle dispersion is $E_{k}^{0} = \sqrt{(\xi_{k}^{0})^{2} + (\Delta_{k}^{S})^{2}}$ with

$$\xi_{k}^{0} = \left(\frac{\epsilon_{k}^{\pm} + \epsilon_{k+Q}^{\pm}}{2}\right) + \eta\sqrt{\left(\frac{\epsilon_{k}^{\pm} - \epsilon_{k+Q}^{\pm}}{2}\right)^{2} + (\Delta_{k}^{S})^{2}} \quad (\eta = 1, \text{ and } -1 \text{ for upper, and lower band}) \quad (2)$$

We take the phenomenological SDW description for representation, which reproduces the hourglass-shape[19], and low-energy commensurate magnetic excitations[17] in hole-doped, and electron doped cuprates, respectively. The other possibility will be also discussed. The model Hamiltonian yields to

$$H = \sum_{k,\sigma}(\epsilon_{k} - \mu) c_{k\sigma}^\dagger c_{k\sigma} - \Delta_{N} \sum_{k,\sigma} \sigma c_{k\sigma}^\dagger c_{k+Q\sigma} \quad (2)$$

Here, $\Delta_{k}^{N} = \Delta_{N}$ is isotropic, representing the strength of the SDW. Its value can be in principle evaluated self-consistently with a reduced Coulomb repulsion $U$ in the mean-field level[25]. Here, we treat it as an independent parameter, determined experimentally. The chemical potential $\mu$ is fixed by the particle conservation. The normal and anomalous Green’s functions are both $2 \times 2$ matrices defined as $\hat{G}_{k\sigma} = -\langle T_{r}\psi_{k\sigma}(\tau)\psi_{k\sigma}^\dagger(\tau) \rangle$, and $\hat{F}_{k} = -\langle T_{r}\psi_{-k\uparrow}(\tau)\psi_{k\uparrow}^\dagger(\tau) \rangle$, where $\psi_{k\sigma} = (c_{k\sigma}, c_{k+Q\sigma})^{T}$. The transversal spin susceptibility under the random phase approximation, also a $2 \times 2$ matrix, is expressed as $\hat{\chi}_{0} = \frac{\hat{\chi}_{0}^{0}}{1 - \chi_{0}^{0}}$ with $U$ the above introduced reduced Coulomb repulsion. $\hat{\chi}_{0}^{0} = -\sum\langle\hat{G}_{k}\hat{G}_{k+Q} + \hat{F}_{k}\hat{F}_{k+Q}^{*}\rangle$ is the bare spin susceptibility, $k \equiv (k, \omega)$.

In order to extract the role of superconductivity on the magnetic excitations, we adopt the difference of spin susceptibility near $Q$ between the SC and normal state as $I_{Q}(\omega) = \int_{Q} \{\chi_{S}(\omega) - \chi_{N}(\omega)\} dq$, consistent with the experimental measurements[7-9]. The integration is restricted within a small window of $0.01\pi \times 0.01\pi$ centered at $Q$ point. The main features are insensitive to the selected integral region. In numerics, the dressed TB parameters up to fourth nearest neighbors, neglecting $t_{z}$, are adopted[26]. It should be emphasized that our results are indeed not sensitive to the selected hoping constant. In the electron-doped cuprates, we only focus on $x = 0.15$, near the optimal doping. The temperature is fixed at $3K$. To highlight the resonance, a broaden factor $\Gamma = 0.2meV$ is adopted.

**Resonance and Fermi surface topology** In Fig. 1, two typical $I_{Q}(\omega)$ in hole-doped cuprates are shown. The spin gap emerges at low enough energy region, reflecting the fact that the magnetic excitations are suppressed due to the opening of SC gap. $I_{Q}(\omega)$ then increases quickly and reaches its maximum at given energy, where the resonance $E_{\text{res}}$ is experimentally defined. These low-energy features are qualitatively consistent with the INS measurements. The resonance energy $E_{\text{res}}$ enhances with increasing SC gap $\Delta_{S}$, well consistent with experimental measurements. Our theoretical data are even quantitatively comparable to the INS measurements[10]. In optimal doping (Fig. 1(b)), the estimated $E_{\text{res}} \sim 22meV$ for $\Delta_{S} = 16meV$, well within the error bar in LSCO. In fact, the resonance energies exhibit a linear dependence on given SC gap (Fig. 3). In optimal doping case, this ratio of the linear scaling $E_{\text{res}}/2\Delta_{S}^{N} = 0.66$, roughly consistent with the measured data $0.51 \pm 0.1$ and experimental proposed universal scaling $0.64[10]$. When the strength of SDW enhances, for example, $\Delta_{N} = 200meV$ at $x = 0.1$ (Fig. 1(a)), the linear dependence remains,
but the ratio $E_{\text{res}}/2\Delta_S^{\text{AN}}$ weakens down to 0.54.

The similar linear scaling can also be found in the electron-doped cuprates both in the monotonic and nonmonotonic d-wave cases as shown in Fig. 2. This suggests the linear dependence of $E_{\text{res}}$ on $\Delta_S$ is a universal feature in the cuprates. The ratio of $E_{\text{res}}/2\Delta_S^{\text{AN}}$ is about 0.69 for $\Delta_N = 150\text{meV}$ in case of the monotonic d-wave, approximately approaching to the suggested value 0.64[10]. In contrast, $E_{\text{res}}/2\Delta_S^{\text{AN}}$ is about 1.73 in case of the nonmonotonic d-wave, exhibiting the strong deviations from 0.64. We notice that the intensity of $I_Q(\omega)$ weakens with decreasing $\Delta_S$. This is well consistent with INS measurements on $PLCCO$, where the external magnetic field is applied to suppress the superconductivity[9].

Interestingly, when the strength of SDW is reduced down to $80\text{meV}$, a weak but visible low-energy peak emerges below $E_{\text{res}}$, especially for the stronger superconductivity (Fig. 2(b) and (d)). This is well comparable with the recent INS data measured by Yu et al. on the optimal doped $NCCO[11]$, where a low-energy peak at $4.5\text{meV}$ is discovered. However, the low-energy peak is absent in another INS measurement on optimal doped $NCCO[7]$. This may be due to not well oxygen annealing in the latter sample, which enhancing the strength of SDW. We also analyze the data with $\Delta_N = 100\text{meV}$ (not shown), where the low-energy resonance peak is almost invisible unless strong enough SC gap is applied. Moreover, the low-energy resonance peak is also not found in optimal doped $PLCCO$, where the SDW is much enhanced due to low doping density ($x=0.12$). This is consistent with the case of $\Delta_N = 150\text{meV}$. We believe the present resonance with two peaks can be further discovered in the slightly overdoped $n$-type cuprates. More INS measurements are expected to check it.

As demonstrated above, our numerical data show that the distinct ratio can be found in the respective case as shown in Fig. 3(a). Typically, $E_{\text{res}}/2\Delta_S^{\text{AN}}$ is about 0.5 ~ 0.7 in the hole-doped cuprates, 0.6 ~ 0.7, and 1.7 for high-energy resonance in the electron-doped cuprates with monotonic, and nonmonotonic d-wave, respectively. While for the low energy resonance, the ratio ranges from 0 ~ 0.55, and 0 ~ 0.9 in case of the monotonic, and nonmonotonic d-wave. This ratio can be even higher when the SDW is further suppressed. The experimentally universal scaling $E_{\text{res}}/(2\Delta_S^{\text{AN}}) \sim 0.64$ seems to be insufficient to cover the whole situations. Whether there still exists a universal scaling between the resonance energy and SC gap, and the intrinsic relation between the resonance and superconductivity are then naturally put forward.

To understand these issues, we have to analyze the magnetic response further. In fact, the main features of the bare spin susceptibility difference $\Delta \chi^0(\omega)$ are almost the same as the RPA one as shown in the left panels in Fig. 4, but with much reduced intensity. For simplicity, we directly analyze $\Delta \chi^0(\omega)$ instead. It includes four components: the intra-band components $I_{Q^+}$ and $I_{Q^-}$,
the inter-band components $I_{Q}^{x+}$ and $I_{Q}^{y-}$. In hole-doped cuprates, $I_{Q}^{x}(\omega)$ fully comes from the intra-band components $I_{Q}^{x-}$ (Fig 4(a)). As well known that the Fermi surface is a hole-pocket due to the lower band $(-)$ crossing the Fermi energy in presence of SDW. It loses most intensity beyond the magnetic Brillouin zone (Fig 4(d)), resulting the well known ‘arc’-type Fermi surface. When we focus on the difference of integration nearby $Q = (\pi, \pi)$, the scattering between the two hot spots contributes the most intensity as denoted by arrows. On the other hand, the SC order parameter changes sign between the two hot spots, which is the essence of the resonance as stressed previously[27]. In electron-doped cuprates, only electron-pocket near antinodes can be found for strong SDW (Fig. 4(e)), which is induced by the upper bands (+). $I_{Q}^{x}(\omega)$ fully comes from the intra-band component $I_{Q}^{x+}$ due to the dominate scattering between the two hot spots. Therefore, only a single resonance peak can be found in the above two cases. However, they come from respective component.

The situation changes when SDW are weakened in the electron-doped cuprates. The hole and electron pocket emerge simultaneously (Fig. 4(f)), consisting with the large three-piece Fermi surface structure found in optimal doped NCCO [28]. Now, there exists two types of scattering between the hot spots. Both intra-band components contribute to $I_{Q}^{x}(\omega)$ as shown in Fig. 4(c). The low-, and high-energy resonance comes from $I_{Q}^{x-}$, and $I_{Q}^{x+}$, respectively. Therefore, the two resonances are related to the $B_{1g}/B_{2g}$ found in the Raman scattering[30]. The low-energy resonance can be covered by the high-energy resonance when SDW enhances slightly, for example $\Delta_N = 100meV$ as we mentioned above, where the component $I_{Q}^{x-}$ is too small to be discovered. This is a possible reason for the absence of the low-energy resonance even in the optimal doped NCCO as discovered by Zhao et al.[7]. The two resonances may also be coincident when SDW is weak enough due to proximity of the two types of hot spots, which is expected to be discovered in the overdoped $n$-type cuprates. Therefore, the features of resonance can be well understood by the scattering between the hot spots induced by the Fermi surface topology.

Reminding the scattering between the hot spots contributes mostly as mentioned in the above analysis. We therefore propose to adopt $E_{res}/2\Delta_S^H$ instead, where $\Delta_S^H$ is the magnitude of the SC gap at the hot spot. There are two types of hot spot in the SDW suppressed electron-doped cuprates. After renormalization, a new scaling with $E_{res}/2\Delta_S^H \sim 1.0$ is well established. This universal scaling is independent on the details, whatever the monotonic/nonmonotonic $d$-wave, hole-/electron-doping, high/low energy resonance, and the selected dressed TB parameters. In fact, it is also model independent if the Fermi surface topology is established. In Fig. 3, we also present the results obtained from DDW and SSC introduced before. The same ratio further manifests that the resonance is rather a consequence of Fermi surface topology. Further INS measurements on various cuprates are expected to justify this universal scaling.

**Resonance and pairing symmetry** To understanding the intrinsic relation between the resonance and superconductivity, we consider two other singlet pairing symmetries: the on-site $s$-wave $\Delta_S^k = \Delta$, and extended $s$-wave $\Delta_S^k = \frac{1}{2}\Delta(\cos k_x + \cos k_y)$. The former is typically found in the conventional superconductor, while the latter is proposed in the recent discovered Fe-pnictides, producing the so-called $s'$-wave nature[29]. No resonance can be found in both two types of pairing symmetry due to the lack of the sign changing of the SC gap between the two hot spots. Therefore, the resonance in cuprates is closely linked to the $d$-wave pairing symmetry.

The monotonic $d$-wave pairing is a consensus in the hole-doped cuprates. However, it is controversial in the
electron-doped cuprates. Both the monotonic and nonmonotonic d-wave are proposed to explain the ARPES data[1]. The resonance in x = 0.12 doped PLCCO is about 11 meV[8]. This means that the SC gap at the antinode should be 7.5 meV, and 3 meV in the monotonic, and nonmonotonic d-wave pairing providing $\Delta_N = 150$ meV, respectively. Matsui et al. revealed that $\Delta^N \approx 2.0$ meV at 8 K by the ARPES measurements[23]. Therefore, the pairing in electron-doped cuprates is more likely a nonmonotonic d-wave. Furthermore, the experimental low-energy resonance peak in optimal doped NCCO is about $E_{res} = 4.2$ meV[11]. It roughly corresponds to the antinodal SC gap about 7 - 8 meV, and 2.2 meV in the monotonic, and nonmonotonic d-wave in case $\Delta_N = 80$ meV. Compared with the Raman scattering measurements[24], the gap along the antinodal direction is merely about 3 meV, corresponding to $\Delta^N \approx 2.2$ meV. We again confirm that the SC pairing in electron-doped cuprates is the nonmonotonic d-wave. The corresponding high-energy peak is about 8.5 meV for $\Delta_N = 80$ meV, consisting with the data obtained by Yu et al., which may underestimate the high energy component in their analysis. More INS measurements are expected to clarify the discrepancy. Therefore, the INS technique can be used to verify the pairing symmetry, and even the details.

The similar scaling $E_{res}/2\Delta \sim 0.64$ had also been suggested in the iron-based superconductor by INS[4]. More recently, a collective boson mode with $E_{res} \sim 2\Delta$ is found by the scanning tunnelling spectroscopy[31]. The hole-pocket, and electron-pocket emerge near (0, 0), and (\pi, \pi) point, where the $s^+$ and $s^-$ wave locate, respectively[29]. Therefore, the dominate contributions are expected to come from the inter-band components. Furthermore, the iron-based superconductors are thought to be analog to the cuprates after a gauge mapping[32]. Our analysis on the cuprates may be further applied to the iron-based superconductors.

In summary, the resonance and its intrinsic links to the superconductivity are studied in cuprates. The main features discovered experimentally are well established. The resonance energy exhibits linear dependence on the SC gap. A low-energy resonance develops in the electron-doped cuprates when SDW is suppressed. The respective resonance comes from the different origins in hole/electron-doped cuprates, and the low-/high-energy resonance in the electron-doped cuprates. We further propose a universal scaling $E_{res}/2\Delta_H \sim 1.0$ instead of the experimentally suggested $E_{res}/2\Delta^{AN} \sim 0.64$, irrespective of the detailed selections. Present work strongly suggested that the resonance is rather a consequence of d-wave pairing nature and Fermi surface topology than the glue of the superconductivity. Based on our analysis, the pairing symmetry in electron-doped cuprates is more likely the nonmonotonic d-wave pairing. Therefore, the resonance in INS measurements is not only related to the pairing symmetry, but also to the detailed form.

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