Gap function symmetry and spin dynamics in electron-doped cuprate superconductor

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An antiferromagnetic (AF) spin fluctuation induced pairing model is proposed for the electron-doped cuprate superconductors. It suggests that, similar to the hole-doped side, the superconducting gap function is monotonic $d_{x^2-y^2}$-wave and explains why the observed gap function has a nonmonotonic $d_{x^2-y^2}$-wave behavior when an AF order is taken into account. Dynamical spin susceptibility is calculated and shown to be in good agreement with the experiment. This gives a strong support to the proposed model.

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I. INTRODUCTION

Pairing symmetry is an important issue towards understanding the mechanism of superconductivity. For hole-doped cuprate high-$T_c$ superconductor, it is generally accepted that the pairing symmetry is $d_{x^2-y^2}$-wave [1]. On the other hand, although no consensus has been reached yet, more and more recent experiments have pointed out that the order parameter of electron-doped cuprate superconductors is also likely to have a $d_{x^2-y^2}$-wave pairing symmetry [2, 3, 4, 5, 6]. Interestingly however, angle resolved photoemission measurement (ARPES) [4] and Raman scattering [5, 6] suggest a nonmonotonic $d_{x^2-y^2}$-wave order parameter with maxima close to the nodes (diagonals) rather than to the Brillouin zone (BZ) boundary. Understanding the origin of the nonmonotonic $d_{x^2-y^2}$-wave order parameter becomes an important issue. Yoshimura and Hirashima performed a strong-coupling one-band calculation and claimed that the nonmonotonic feature comes from a strong AF spin fluctuation [7]. In contrast to hole-doped cases, they [7] found that the hot spots, the intersections of the magnetic BZ boundary and the Fermi surface (FS), are located near the diagonals of the BZ. Alternatively it was also argued that the nonmonotonic feature of the order parameter is the outcome of the coexistence of the superconducting (SC) and the AF orders [8, 9, 10]. When AF order coexists with the SC order, the resulting quasiparticle (QP) excitation can be gapped by both orders and the SC gap itself could have a typical monotonic $d_{x^2-y^2}$ symmetry.

The clue to understand the electron doped cuprate comes from two doping-dependent FS as revealed by ARPES [11, 12]. These are well explained in terms of the $k$-dependent band-folding effect associated with an AF order which splits the band into upper- and lower-branches [13, 14]. In the SC state, the QPs could pair each other within the same band that leads naturally to a two-band/two-gap model. The two-gap model gives a unified explanation for the upward feature near $T_c$ and the weak temperature dependence at low $T$ in superfluid density $\rho_s$ [15]. It is also supported by Hall coefficient and magneto-resistance measurements [16, 17, 18].

Raman scattering has the potential to probe different regions of the FS. It has been shown by Lu and Wang [9] that SC and AF orders in electron-doped cuprates are disentangled in Raman spectra. In our earlier calculation on Raman spectra [12], we have also proved that the Raman shift for electron-doped cuprates is mainly determined by their pair breaking associated with different pieces of the FS. The AF order can cause a vertex correction and enhance the spectral weight, but nevertheless, it does not change the Raman symmetry. In particular, near the optimally-doped regime, the frequency of $B_{3g}$ peak appears to be higher than that of $B_{1g}$ peak [5, 6]. It seems indicating that the SC gap deviates from the monotonic $d_{x^2-y^2}$-wave. However, it has been shown that it is indeed two monotonic $d_{x^2-y^2}$-wave gaps, associated with $\alpha$ and $\beta$-band FS respectively, which leads to a good description for it [19].

In this paper, spin dynamics is explored to further test the two-gap model for the electron-doped cuprates. Spin fluctuation is observable by inelastic neutron scattering (INS), and is confirmed to be intimately connected with the pairing mechanism in hole-doped cuprates. In single (CuO$_2$) layer hole-doped cuprates such as La$_{2-x}$Sr$_x$CuO$_4$, the magnetic peak is always incommensurate and their incommensurability is robust against the frequency change [20, 21]. (Strong commensurate peak at momentum $Q \equiv (\pi, \pi)$ and some particular resonance frequency $\omega_r$ has been observed in multilayer YBa$_2$Cu$_3$O$_7$ and Bi$_2$Sr$_2$CaCu$_2$O$_8$ though [22] ) In current single-layer electron-doped cuprates such as Nd$_{2-x}$Ce$_x$CuO$_4$ (NCCO), in contrast, commensurate peak at $Q$ is observed both in the SC and normal states [23, 24, 25, 26]. These commensurate peaks survive over a wide frequency range. It will be shown later that the commensurability of these magnetic peaks is a natural outcome of the band nesting, and their robustness is actually incorporated into the existence of two separate bands. Spin dynamics has been theoretically examined in various aspects for electron-doped cuprates lately [27, 28, 29, 30].

Based on a mechanism making use of the strong AF spin fluctuation, a pairing model will be proposed for the
electron-doped cuprates. Analogous to the hole-doped side, the SC gap function of the electron-doped cuprates is thus naturally to have the $d_{x^2−y^2}$ symmetry in the whole doping range. When the AF order is significant, it makes a big split between the two bands and consequently the nonmonotonic $d_{x^2−y^2}$-wave like of the gap is satisfactorily explained. Of equal importance, this model gives a unified picture for the Raman scattering, $\rho_s(T)$, and INS in electron-doped cuprates.

II. THE MODEL

We start with a phenomenological superconducting Hamiltonian

$$H = \sum_{k,\sigma} \left[ \varepsilon_k f_{k,\sigma}^\dagger f_{k,\sigma} + \Delta_k \left( f_{k,\sigma}^\dagger f_{-k,\uparrow} + f_{-k,\downarrow} f_{k,\sigma} \right) \right]$$

$$ - 2Jm \sum_{k,\sigma} \sigma (f_{k,\sigma}^\dagger f_{k+Q,\sigma} + \text{h.c.}) - \mu$$

originated from a $t$-$t'$-$J$ model. The slave-boson transformation and spin-density-wave mean-field approximation are undertaken. Here $f_{k,\sigma}^\dagger$ ($f_{k,\sigma}$) is the fermionic spinon creation (destruction) operator, $m = (-1)^i(S_i^z)$ is the AF order, $\mu$ is the chemical potential, and

$$\varepsilon_k = (2|t|\delta - J\chi)(\cos k_x + \cos k_y) - 4t'\delta \cos k_x \cos k_y - 2t''\delta(\cos 2k_x + \cos 2k_y)$$

is the independent particle dispersion with $\delta$ the doping concentration and $\chi = \langle f_{\sigma}^\dagger f_{\sigma} \rangle$ the uniform bond order. The prime denotes that momentum summation is over the magnetic BZ only ($-\pi \leq k_x \pm k_y \leq \pi$). The SC gap function is given self-consistently

$$\Delta_k = \sum_{k'} V(k, k') \langle f_{k',\uparrow}^\dagger f_{k',\downarrow} \rangle ,$$

where $V(k, k')$ is the pairing potential. Using the unitary transformation

$$\begin{pmatrix} f_{k,\sigma} \\ f_{k+Q,\sigma} \end{pmatrix} = \begin{pmatrix} \cos \theta_k & \sin \theta_k \\ \sin \theta_k & \cos \theta_k \end{pmatrix} \begin{pmatrix} \alpha_{k,\sigma} \\ \beta_{k,\sigma} \end{pmatrix}$$

with $\theta_k$ being defined by $\tan 2\theta_k = 4Jm/[\sigma(\varepsilon_k+Q-\varepsilon_k)]$, Hamiltonian (1) can be transformed as [31, 32]

$$H = \sum_{k,\sigma} \left[ \xi_k \left( f_{k,\sigma}^\dagger f_{k,\sigma} \right) + \Delta_k \left( f_{k,\sigma}^\dagger f_{-k,\uparrow} + f_{-k,\downarrow} f_{k,\sigma} \right) \right] - \mu l,$$

where $l = \alpha, \beta$, $\mu_a + \mu_\beta = \mu$, and

$$\xi_k \equiv \varepsilon_k + \varepsilon_k + Q \pm \sqrt{(\varepsilon_k+Q-\varepsilon_k)^2/4} + 4J^2m^2$$

corresponding to the QP (with only the AF order in it) dispersions of the two ($\alpha$ and $\beta$) bands.

III. GAP SYMMETRY: MONOTONIC VS. NONMONOTONIC $d_{x^2−y^2}$-WAVE

As mentioned previously, ARCES [4] and Raman [5] reveal the gap function $\Delta_k$ in electron-doped cuprate SC to have a non-monotonic $d_{x^2−y^2}$-wave like. For example in Ref. [33], $\Delta_k \equiv \Delta_0 \gamma_k$ with $\gamma_k = \sin 2\phi + a_1 \sin 4\phi + a_2 \sin 6\phi$ ($\phi$ being the angle measured relative to the diagonal on the FS) was used to simulate a non-monotonic $d_{x^2−y^2}$-wave gap [see also Fig. (1b)]. In this kind of approaches, parameters $a_1$ and $a_2$ are doping dependent.

As far as SC gap is concerned, it is physically more appealing that $\gamma_k$ remains the same for the entire doping
TABLE I: Parameters used to calculate $\Delta_{\alpha}$ and $\Delta_{\beta}$.

| $\delta$ | $m$ | $-\gamma$ | $-\mu_{\alpha}$ | $\mu_{\beta}$ |
|---------|-----|-----------|-----------------|---------------|
| 0.15    | 0.178 | 0.15      | 0.005           | 0.078         |
| 0.155   | 0.169 | 0.16      | 0.007           | 0.079         |
| 0.16    | 0.160 | 0.17      | 0.008           | 0.079         |
| 0.165   | 0.150 | 0.18      | 0.009           | 0.079         |
| 0.17    | 0.040 | 0.20      | -0.040          | -0.036        |
| 0.18    | 0.010 | 0.20      | -0.034          | -0.035        |

range, so long as the pairing mechanism remains the same (no quantum criticality occurs). Based on a mechanism induced by the strong AF spin fluctuation, we propose the following piecewise model for the pairing potential

$$V(k, k') = \begin{cases} 
  g_{\alpha} \gamma_k \gamma_{k'}, & \text{for } k, k' \text{ on } \alpha\text{-band FS}, \\
  g_{\beta} \gamma_k \gamma_{k'}, & \text{for } k, k' \text{ on } \beta\text{-band FS}, \\
  0, & \text{otherwise,}
\end{cases} \quad (7)$$

where $\gamma_k = \sin 2\phi$, and $g_{\alpha}$ and $g_{\beta}$ are the two coupling constants. Inspired by the hole-doped side, it is promisingly to have $\gamma_k$ having the monotonic $d_{x^2-y^2}$ symmetry. This is strongly supported by the INS experiment and will be elaborated later. Nevertheless, there are two $d_{x^2-y^2}$-wave gaps, possibly with different amplitude, for the current electron-doped side. When AF order breaks down with increasing the doping, the two bands [Eq. (6)] will eventually merge into a single one. In this regime, the behavior of the electron-doped cuprates is expected to be very similar to that of the hole-doped ones, with one single monotonic $d_{x^2-y^2}$-wave gap [19]. The latter is confirmed by the Raman experiment [13].

The piecewise feature in $V(k, k')$ comes naturally for the AF spin fluctuation induced mechanism (see Sec. IV). Only QPs within the same band favor the pairing associated with the $Q$ wavevector . This is also supported by the superfluid data which unambiguously reveals that QPs in $\alpha$ (or $\beta$) band FS pair each other to form SC QPs. But no SC QP forms in the region where FS is absent [16].

Substitution of (7) and (4) into (3), one obtains the self-consistent gap equation respectively for each band

$$1 = g_l \sum_{k \in \alpha\text{-FS}} \gamma_k^2 \tanh \left( \frac{E_{k\ell}}{2k_BT} \right), \quad (8)$$

where $E_{k\ell} = \sqrt{\varepsilon_k^2 + \Delta_{\ell}^2}$ and $\Delta_{k\ell} = \Delta_{\ell} \gamma_k$. In practice, the $k$ sum in (8) can be effectively extended to the whole MBZ because contribution due to the $k$ points distant from the corresponding $l$-band FS is negligible. Fig. (1b) shows an example of piecewise monotonic $d_{x^2-y^2}$-wave $\Delta_{k\ell}$, compared with a nonmonotonic one. The region between $(\phi_{\alpha}, \phi_{\alpha})$ is where FS is absent and no SC gap associated with.

Shown in Fig. (1c) are the two gap amplitudes, $\Delta_{\alpha}$ and $\Delta_{\beta}$, calculated at $T = 0$ with various doping levels. As the doping $\delta$ decreases (and hence the AF order $m$ increases), the ratio of $\Delta_{\beta}/\Delta_{\alpha}$ increases along with the gapped $(\phi_{\beta}, \phi_{\alpha})$ region opens up. This manifests the non-monotonic $d_{x^2-y^2}$-wave like gap nicely. Both $\Delta_{\alpha}$ and $\Delta_{\beta}$ decrease as doping increases. At over doping ($\delta \geq 0.17$), $m$ approaches zero and FSs join to one piece, $\Delta_{\alpha}$ and $\Delta_{\beta}$ match. These consistent results give strong support to the model pairing [7]. The parameters used are listed in Table I. Coupling constants, $g_{\alpha}$ and $g_{\beta}$, are fixed at 0.34 and 0.62 respectively, that give the best fit for optimal doping ($\delta = 0.15$). Fig. (1d) displays the temperature dependence of $\Delta_{\alpha}$ and $\Delta_{\beta}$ ($\delta = 0.15$). The SC $T_c$, determined by the higher of the onset temperatures that make $\Delta_{\alpha}$ or $\Delta_{\beta}$ vanish, is found to be about 25 K. The two onset temperatures, differed by 4K or so, are in good agreement with the upward curvature observed in $\rho_s$ near $T_c$ [12].

IV. DYNAMICAL SPIN SUSCEPTIBILITY

The dynamical spin susceptibility, which comes from the particle-hole excitations, is given by

$$\chi^0(q, \omega) = \frac{1}{N} \langle T_{\tau} S^z_q(\tau) S^z_{-q}(0) \rangle_0, \quad (9)$$

where $S^z_q = \frac{1}{2} \sum_{k, \sigma} f_{k+q/2, \sigma} f_{k-q/2, \sigma}$ is the spin-density operator with $\sigma$ the spin index. Using the transformation (4) and Fourier transforming $\chi^0(q, \tau)$ into the Matsubara frequency space, one obtains

$$\chi^0(q, i\omega_n) = -\frac{1}{2N} \sum_{k, \ell'} \nu_{k, \ell'} \chi^0_{k, \ell'}(q, i\omega_n). \quad (10)$$

Here $\nu_{k, \ell'}(q) = \{1 + \epsilon_{\ell'} \cos[2(\theta_k - \theta_{k+q})]\} \epsilon_{\ell'} = 1 (-1)$ for $l' (l \neq l')$ and

$$\chi^0_{k, \ell'}(q, i\omega_n) = -\frac{1}{\beta} \sum_{\omega_{n'}} \langle G_l(k, i\nu_n) G_{l'}(k + q, i\nu_n + i\omega_n) \rangle + \epsilon_{ll'} F_l(k, i\nu_n) F_{l'}(k + q, i\nu_n + i\omega_n)$$

with $G_l$ and $F_l$ the single-particle normal and anomalous Green’s function of band $l$. Considering the AF vertex correction under the random-phase approximation, one then has the renormalized spin susceptibility $\chi(q, i\omega_n) = \chi^0(q, i\omega_n)/(1 + \nu J(q))$, where $J(q) = \cos(q_y) + \cos(q_x)$ and $\nu$ is the coupling strength. The INS intensity, $I(q, \omega)$, is proportional to $\text{Im}\chi(q, i\omega_n \rightarrow \omega + i0^+)$ As a matter of fact, vertex correction leads to enhancement of the spectral intensity, but giving no qualitative change in the lineshape.

Fig. (2a) shows the calculation of $I(q, \omega)$ with different frequencies ($\omega = 3, 5, 10$ meV) at $T = 0$ and optimal doping ($\delta = 0.15$). The momentum is scanned along the direction of $(0, 0) \rightarrow (\pi, \pi)$. For easy comparison, the coupling strength $\nu$ is chosen to be 0.627, same as that used in Ref. [23]. The most remarkable feature is that $I(q, \omega)$ is commensurate for $\omega \leq 5$ meV, consistent with the INS measurements of Yamada et al. [23]. In the case
FIG. 2: (a) Constant \( \omega \), \( \mathbf{q} \)-dependent INS intensity, \( I(\mathbf{q}, \omega) \), calculated for optimally-doped (\( \delta = 0.15 \), \( T_c = 18K \)) sample in the SC state (\( T \to 0 \)). The smearings are taken to be \( \Gamma_\alpha = \Gamma_\beta = 20 \) cm\(^{-1} \). (b) Energy contours of \( E_k = 2.5 \) meV (5 meV) shown in the second and fourth (first and third) quarters of the BZ. The double-arrow lines denote the corresponding nesting wavevectors. (c)&(d) Comparison between theoretical calculations (solid lines) and experimental data (dots with error bars) of \( I(\mathbf{Q}, \omega) \) on SC NCCO (\( \delta = 0.15 \)). \( T_c = 18 \) and 25 K for (c) & (d).

of higher \( \omega = 10 \) meV, in contrast, \( I(\mathbf{q}, \omega) \) becomes incommensurate. The above theoretical results are in great contrast to those obtained based on a one-band model [28], where spin response is found to be incommensurate at lower frequencies but shifted to be commensurate at higher frequencies.

The switch from a commensurate to the incommensurate peaks upon frequency increase can be understood in terms of the band nesting effect. As illustrated in Fig. 2(b), two sets of energy contours: \( E_k = 2.5 \) meV and 5 meV are plotted respectively in the second and fourth and first and third quarters of the BZ. When energy is low, only \( \beta \) band opens up a contour, and the flat (nesting) portion of the energy contours show a thin strip near the MBZ border. The corresponding wave vector \( \mathbf{q} \) (double arrow) which brings the nesting portion into good alignment with its partner in the other quadrant equals to \( \mathbf{Q} \). Consequently, the nearly degenerate excitations give a commensurate peak. When energy is high, in contrast, both \( \alpha \) and \( \beta \) bands open up a contour. In addition to \( \mathbf{Q} \) nestings, the most contribution may come from the incommensurate \( \mathbf{Q} \pm \delta \) nestings [see Fig. 2(b)].

The exact or near (\( \delta \) is small) \( \mathbf{Q} \) spin fluctuations may assist the QPs to form the \( d_{x^2-y^2} \)-wave pairing. This is the scenario widely believed for the hole-doped side. Based on this pairing mechanism and taking possible \( \mathbf{Q} \) connections into account [in view of Fig. 2(b)], the validity of the model pairing potential [7] is justified.

One can examine the intensity at \( \mathbf{q} = \mathbf{Q} \) more carefully. At low \( \omega \), \( I(\mathbf{Q}, \omega) \) is weak, indicating that a spin gap opens up. \( I(\mathbf{Q}, \omega) \) will reach its maximum at \( \omega = 2\Delta \) with a pairing-breaking gap estimated to be \( |\Delta|^2 \approx 2 \int_{0}^{\delta_0^0} |\Delta_{\mathbf{k}\mathbf{Q}}|^2 d\phi + \int_{\delta_0}^{\delta_0^1} |\Delta_{\mathbf{k}\mathbf{Q}}|^2 d\phi \). When \( \omega \) is higher, nesting portions move out of the MBZ boundary, and consequently \( I(\mathbf{Q}, \omega) \) starts to diminish. A good agreement between the theoretical calculation and experimental \( I(\mathbf{Q}, \omega) \) is obtained and shown in Fig. 2(c)&(d). In Fig. 2(c) with \( T_c = 18K \), \( \Delta_\alpha = 22 \) cm\(^{-1} \) and \( \Delta_\beta = 38 \) cm\(^{-1} \), and \( 2\Delta \approx 5.2 \) meV is obtained. While in Fig. 2(d) with \( T_c = 25K \), \( \Delta_\alpha = 32 \) cm\(^{-1} \) and \( \Delta_\beta = 55 \) cm\(^{-1} \), and \( 2\Delta \approx 7.6 \) meV is given. It is noted that the above \( \Delta_\alpha \) and \( \Delta_\beta \) are taken exactly the same as those led to good fits for the Raman scattering [19].

Recently, high-energy spin excitation of INS experiment is also reported [20]. The energy taken in those experiment is far above \( 2\Delta_1 \) (\( \sim 10 \) meV), beyond the scope of the present paper. In such case, the excitation leads to a spin-wave-like ring [26], and the effect of pairing breaking is weak. A two-dimensional AF Heisenberg model including nearest (\( J_1 \)), next-nearest (\( J_2 \)), and next-next-nearest (\( J_3 \)) couplings should be used to interpret the experiments.

V. SUMMARY

In summary, the gap symmetry of electron-doped cuprate superconductors is studied based on a two-gap model. Considering a mechanism induced by the AF spin fluctuation, a piecewise pairing potential is proposed to account for the observed nonmonotonic \( d_{x^2-y^2} \)-wave feature of the gap. Dynamical spin susceptibility is calculated and shown to be in good agreement with the experiment. This gives a strong support to the proposed pairing model.

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