Momentum dependence of pseudo-gap and superconducting gap in variation theory

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Abstract. To consider the origin of a pseudo-gap and a superconducting gap found in the high-$T_c$ cuprates, the momentum dependence of the singlet gap parameter and the superconductivity correlation function are evaluated in the $t$–$J$ model by using an optimization variational Monte Carlo method. In the underdoped regime, the singlet gap is significantly modified from the simple $d_{x^2−y^2}$-wave gap ($\propto \cos k_x − \cos k_y$) by the contributions of long-range pairings. Its angular dependence along the Fermi surface is qualitatively consistent with those experimentally observed in both hole- and electron-doped cuprates. This singlet gap will correspond to the pseudo-gap and its doping dependence agrees with that of the pseudo-gap. On the other hand, the superconductivity correlation function is dominant in the nearest-neighbor pairing and its Fourier transform preserves the original simple $d_{x^2−y^2}$-wave form. We argue that this superconductivity correlation function is closely related to the coherent superconductivity gap appearing below $T_c$ in the ‘Fermi arc’ region. Its doping dependence is also consistent with the recent experimental observations.

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1. Introduction

Recent experiments of high-$T_c$ cuprates show that the excitation gap structures both above and below the transition temperature, $T_c$, are anomalous compared with the conventional superconductors [1]–[5]. This behavior will be closely related to the mechanism of high-$T_c$ superconductivity (SC) and probably to the physics close to the Mott insulator.

Raman scattering for HgBa$_2$CuO$_{4+\delta}$ [1] and angle resolved photoemission spectroscopy (ARPES) for Bi$_{2212}$ [2], Bi$_{2201}$ [3] and La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) [4, 5] claimed the existence of two gaps: one is near the nodal points, $k \sim (\pm \pi/2, \pm \pi/2)$ on the Fermi surface, and the other is near the antinodal points, $k \sim (\pi, 0)$ and $(0, \pi)$. Furthermore, they exhibit opposite $\delta$ (doping rate)-dependences. The gap in the antinodal region is a well-known pseudo-gap that exists already above $T_c$, and increases as $\delta$ decreases. On the other hand, the gap in the nodal region is considered to be more directly related to the SC, since the gap amplitude decreases as $\delta$ decreases corresponding with the behavior of $T_c$ [6]. Scanning tunneling microscopy (STM) [7] has also found a similar two-gap behavior. If these two gaps in the antinodal and nodal regions are simply assigned to a pseudo-gap ($\Delta_{PG}$) and an SC gap ($\Delta_{SC}$), respectively, the origin of the two gaps can be considered distinct, namely the origin of the pseudo-gap is not related to SC, i.e. not a precursor of SC or SC fluctuation. Actually, very recent experimental studies of ARPES and STM [8] for Bi$_{2201}$ found that two kinds of gaps coexist near the antinodal point: one of the gaps is related to $\Delta_{SC}$ and the other may be of other origin such as charge inhomogeneity. Theoretically, this kind of two-gap feature has been discussed phenomenologically [9] and also numerically using the Hubbard model [10, 11]. Although these results seem to be consistent with experiments, the two different numerical studies do not agree with each other on the point whether the pseudo-gap above $T_c$ survives or not in the superconducting state [10, 11].

Experimentally, it is also claimed that there exists a ‘Fermi arc’, defined as a portion of Fermi surface with finite quasiparticle peak above $T_c$, and that the SC gap, $\Delta_{SC}$, appears in this ‘Fermi arc’ region below $T_c$. Although this picture seems to support the two-gap features, the spread in momentum space of such low energy excitations should be addressed with care by taking account of effects of experimental conditions of both finite temperature and finite energy resolution in ARPES. Actually, there is a claim that the ‘Fermi arc’ shrinks to a point as $T \rightarrow 0$ [12]. If this is the case, the pseudo-gap state at $T = 0$ is a nodal liquid in which there are gapless excitations only at points near $(\pm \pi/2, \pm \pi/2)$ just as in the $d_{x^2-y^2}$-wave SC. In this sense, the relationship between the possible new energy gap associated with SC below $T_c$ and preexisting pseudo-gap is one of the most interesting issues in high-$T_c$ SC.

Furthermore, it has been known that the excitation gap structure in the momentum space more or less deviates from the simple $d_{x^2-y^2}$-wave function of nearest-neighbor-site pairing
(x cos k_x - cos k_y) in some cases. In Bi2212, for example, the angular dependence of the gap becomes concave near the nodal point [13, 14], which is different from the linear dependence in the simple d_{x^2-y^2}-wave function. In the electron-doped systems, the modification is much more significant. It is found that the maximum of the gap is located midway between the Brillouin-zone boundary (π, 0) and the zone diagonal (π/2, π/2) [15, 16], which again differs markedly from the simple d_{x^2-y^2}-wave. Although it is unclear whether Δ_{SC} or Δ_{PG} mainly contributes to these deformed gaps, it is important to elucidate the origin of these modifications in the momentum space.

With this in mind, we discuss in this paper the difference of the momentum dependence of two kinds of physical quantities, i.e. the singlet gap parameter, Δk, optimized in a correlated SC state or a projected Bardeen, Cooper and Schrieffer (BCS) wave function [17], and the Fourier transform of SC correlation function P(τ). We consider the t–J model on the square lattice with second- and third-neighbor hoppings (t–t′–t″–J model) to be fit for the Fermi surface observed by ARPES [18]. This model represents the strongly correlated regime of the Hubbard model and enables us to study the two-gap features from a different viewpoint. In the t–J model, we study variational ground states, using an optimization variational Monte Carlo (VMC) method that accurately gives expectation values of many-body functions. Although finite-temperature behavior is very difficult to discuss, it will be important to study the ground state in a reliable numerical method that can be applied even to the strongly correlated systems. We consider that the singlet gap parameter, Δk, represents the pseudo-gap Δ_{PG} [19] since Δk is the excitation gap of spinons in the slave-boson mean-field theory. This excitation gap can survive above T_c when the holons become incoherent. On the other hand, we expect that the coherent SC gap, Δ_{SC}, appearing below T_c is determined from the SC correlation function, P(τ), although it is not explicitly proved.

In the following, we introduce the long-distance singlet pairs in Δk and show that the optimized gap parameter Δk reproduces the angular dependence of gap functions observed experimentally both for the hole- and electron-doped cuprates. In contrast, the Fourier transform of the SC correlation function, P(τ), looks very similar to the simple d_{x^2-y^2}-wave order parameter. Furthermore, the doping-dependences of Δk and P(τ) are consistent with the recent experimental observations of Δ_{PG} and Δ_{SC}.

2. Model Hamiltonian and variational wave functions

As a model for the CuO2 plane in high-Tc cuprates, we consider the t–J model, which is the most reasonable simplified model for the cuprates [18, 20, 21]:

\[
H = - \sum_{(i,j)\sigma} t_{ij} P_G (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) P_G + J \sum_{(i,j)} (S_i \cdot S_j - n_i n_j/4),
\]

where \( P_G \) is the Gutzwiller projection operator, \( P_G = \prod_{j} (1 - n_j \uparrow n_j \downarrow) \), excluding doubly occupied states from the wave function, and \( t_{ij} \) are first-, second- and third-nearest neighbor hoppings between \( i \) and \( j \) sites [21]. The superexchange interaction, \( J \), is between the nearest-neighbor Cu spins, which acts when the doped carriers (forming Zhang–Rice singlet [20]) are not located on both sites of \( i \) and \( j \). It has been shown that the t–J-type model has a superconducting ground state with d_{x^2-y^2}-wave symmetry in the various approaches, such as VMC simulations [22]–[25], exact diagonalization methods [26] and high-temperature
expansion studies [27, 28]. (Note that the exact treatments like the quantum Monte Carlo methods have not been successful in the two-dimensional \( t-J \) model.)

For the hole-doped case or less-than-half-filling case, we use \( J/t = 0.3 \) (\( t \) being the nearest-neighbor hopping), \( t'/t = -0.16 \) (second-nearest-neighbor hopping), and \( t''/t = 0.20 \) (third-nearest-neighbor hopping) as typical parameterization for YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) (YBCO), and \( t'/t = -0.10 \) and \( t''/t = 0.10 \) for LSCO [21]. We find that it is crucial for the present problem to include the \( t'' \) term. For the electron-doped case or more-than-half-filled case, we apply a particle–hole transformation, \( c^\dagger_j \sigma \rightarrow \exp (i \mathbf{Q} \cdot \mathbf{r}_j) h_{j\sigma} \), with \( \mathbf{Q} = (\pi, \pi) \). Using this transformation, we can study the electron-doped case by the less-than-half-filled model with \( t' \rightarrow -t' \) and \( t'' \rightarrow -t'' \). For example, we use \( t'/t = 0.16 \) and \( t''/t = -0.20 \) for Nd\(_{2-x}\)Ce\(_x\)CuO\(_4\) (NCCO).

To this model, we apply an optimization VMC method [29], which accurately treats the local constraint due to \( P_G \) [24, 25]. As a variational wave function, we extend the Gutzwiller-projected BCS wave function as follows [17, 19, 24, 25]:

\[
\Psi = P_G \left( \sum_k \phi_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right)^{N_e/2} |0\rangle,
\]

where \( N_e \) is the electron number and \( \phi_k \) is the ratio of BCS coefficients:

\[
\phi_k = \frac{v_k}{u_k} = \frac{\Delta_k}{\tilde{\varepsilon}_k - \varepsilon + \sqrt{ (\tilde{\varepsilon}_k - \varepsilon)^2 + \Delta_k^2 }},
\]

with

\[
\tilde{\varepsilon}_k = -2t (\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - 2t'' (\cos 2k_x + \cos 2k_y).
\]

Variational parameters to be optimized are a singlet gap parameter, \( \Delta_k \), chemical potential, \( \varepsilon \), and band renormalization parameters \( \tilde{t}'/t \) and \( \tilde{t}''/t \). Note that \( \tilde{t}'/t \) and \( \tilde{t}''/t \) are optimized independently of \( t'/t \) and \( t''/t \) in the Hamiltonian equation (1). These renormalizations are important [30] since they deform the Fermi surface and stabilize \( d_{x^2-y^2}\)-wave SC or antiferromagnetic (AF) long-range ordered state, by retrieving the nesting condition of \( (\pi, \pi) \) [30]–[34].

In this paper, we extend the previous VMC calculations [24, 25] by introducing long-range Cooper pairings in \( \Delta_k \). Preserving the \( d_{x^2-y^2}\)-wave symmetry, we extend the variational singlet gap \( \Delta_k \) as

\[
\Delta_k^{\text{ext,d}} = \sum_{n=1}^{4} \Delta_d^{(n)} (\cos nk_x - \cos nk_y)
\]

\[
+ \Delta_d^{(5)} \left[ \cos (2k_x + k_y) - \cos (k_x + 2k_y) \right]
\]

\[
+ \Delta_d^{(6)} \left[ \cos (2k_x - k_y) - \cos (k_x - 2k_y) \right]
\]

\[
+ \Delta_d^{(7)} \left[ \cos (3k_x + k_y) - \cos (k_x + 3k_y) \right]
\]

\[
+ \Delta_d^{(8)} \left[ \cos (3k_x - k_y) - \cos (k_x - 3k_y) \right],
\]

where \( \Delta_d^{(n)} \) are variational parameters as shown in figure 1. \( \Delta_d^{(n)} \) with \( n = 2-4 \) are longer-range pairings in the axis directions and those with \( n = 5-8 \) in oblique directions. The relations \( |\Delta_d^{(5)}| = |\Delta_d^{(6)}| \) and \( |\Delta_d^{(7)}| = |\Delta_d^{(8)}| \) must hold, but their signs can be generally different. We
Figure 1. Variational singlet order parameters, $\Delta^{(n)}_d$, are shown schematically in real space. The Cooper pairs can be considered to be located between the origin (solid circle) and the site $n$ ($n = 1–8$) with the magnitude $\Delta^{(n)}_d$. As an example, the extent of the pair wave function in the case of $n = 5$ [$\Delta^{(5)}_d$] is illustrated by open lobes (minus sign) and hatched lobes (plus sign), which preserve the $d_{x^2-y^2}$-wave symmetry.

optimize these gap parameters independently to allow the difference of the signs. Note that $\Delta^{\text{ext},d}_k$ is reduced to the simple $d_{x^2-y^2}$-wave pairing when $\Delta^{(n)}_d = 0$ for $n = 2, 3, \ldots, 8$. Generally speaking, even if the Hamiltonian has only nearest-neighbor interactions, its ground-state wave function can have long-range $\Delta^{(n)}_d$, which is in sharp contrast to the mean-field theory. One might think that the long-range Coulomb repulsion can have strong effects on $\Delta^{(n)}_d$. However, near the half-filling where only a small number of holes exist, the charge fluctuation is suppressed due to the Gutzwiller projection, and the long-range Coulomb repulsion has little effect. Note also that, in the present calculation, we do not take account of the coexistence of antiferromagnetism with SC observed experimentally [35], which will be important in the very vicinity of half-filling [36].

In the present VMC method, a simple linear optimization of each parameter with fixing the other parameters is employed according to the optimization VMC procedure [29]. In one round of iteration, every parameter is once optimized in one dimension, with $2–5 \times 10^4$ Monte Carlo samples. Then we average the results of the 10–20 rounds after convergence, and determine the optimized variational parameters and the variational energy. Therefore, our data are substantially the averages of $2–10 \times 10^5$ samples, and the statistical errors in energy are suppressed down to the order of $10^{-4}t$. Physical quantities are calculated using the optimized parameters with $2–5 \times 10^4$ samples. The systems used are of $N_s = L \times L$ sites with periodic–antiperiodic boundary conditions. We study the systems with $L = 12–14$ to check the system-size dependence.

3. Singlet gap parameters and SC correlation functions

Figure 2 shows the optimized gap parameters $\Delta^{(n)}_d$ ($n = 1–8$) as a function of doping concentration, $\delta$, for the three parameter sets discussed above. In all cases, the magnitude of the
Figure 2. Optimized singlet gap parameters $\Delta_{d}^{(n)}$ and spin structure factor $S(Q)$ with $Q = (\pi, \pi)$ as a function of doping concentration, for three parameter sets: (a) $t'/t = -0.10$ and $t''/t = 0.10$ of LSCO, (b) $t'/t = -0.16$ and $t''/t = 0.20$ of YBCO and (c) $t'/t = 0.16$ and $t''/t = -0.20$ of NCCO. The data obtained in the system sizes of $L = 12$ and 14 are plotted simultaneously.

The nearest-neighbor gap parameter, $\Delta_{d}^{(1)}$, is always far larger than the other $\Delta_{d}^{(n)}$, supporting the simple $d_{x^2-y^2}$-wave assumption as a first approximation [22, 23]. $\Delta_{d}^{(1)}$ increases monotonically as $\delta$ decreases except for the vicinity of half-filling, $0 \lesssim \delta \lesssim 0.05$, in the hole-doped cases (figures 2(a) and (b)). The overall $\delta$-dependence is similar to that of the observed pseudo-gap [2, 3, 4, 6]. In figure 2, we also compare the gap parameter with spin structure factor, $S(q)$, at the AF wave number $q = Q = (\pi, \pi)$. For all the parameter sets, $S(Q)$ behaves similarly to $\Delta_{d}^{(1)}$, suggesting a close relationship between the AF correlation and the formation of nearest-neighbor singlet pairings. Incidentally, the decrease of $\Delta_{d}^{(1)}$ in the vicinity of half-filling is probably caused by the retrieval of nesting condition. For example, $\Delta_{d}^{(1)}$ for the hole-doped case of $t'/t = -0.16$ and $t''/t = 0.20$ (figure 2(b)) is smoothly connected to that for the electron-doped case of the identical parameter sets, namely $t'/t = 0.16$ and $t''/t = -0.20$ (figure 2(c)).

Let us discuss the long-range gap parameters for the two hole-doped cases shown in figures 2(a) and (b). In these cases, the long-range $\Delta_{d}^{(n)}$ have small but finite values. In particular, $\Delta_{d}^{(2)}$ has appreciable values of $0.1-0.2$. Furthermore, $\Delta_{d}^{(3)}$, $\Delta_{d}^{(5)}$ and $\Delta_{d}^{(6)}$ are also finite in the range of $\delta \lesssim 0.2$ for $t'/t = -0.10$ and $t''/t = 0.10$ (figure 2(a)), and $\delta \lesssim 0.3$ for
$t'/t = -0.16$ and $t''/t = 0.20$ (figure 2(b)). The energy gain introduced by these long-range components with respect to the pure $d_{x^2-y^2}$-wave form is about $0.0004t \pm 0.0002t$ for most of the parameters we used. For example, the variational energies with and without long-range components are $E/t = -0.5979$ and $-0.5975$, respectively, for a typical hole-doped case with $J/t = 0.3$, $t'/t = -0.16$, $t''/t = 0.20$ and $\delta = 0.139$ in the $12 \times 12$-site system. Although the energy gain is small, it is always larger than the statistical errors.

The long-range components $\Delta_0^{(n)}$ deform the simple $d_{x^2-y^2}$-wave gap function. Actually, figure 3 shows angular dependences of the optimized $\Delta_{\mathbf{k}}^{\text{ext.d}}$ along the Fermi surface for several values of doping concentration. Here, the Fermi surface is determined from the tight-binding band $\tilde{E}_\mathbf{k}$ with the optimized band-renormalization parameters, $\tilde{t}'/t$ and $\tilde{t}''/t$, for each parameter set. Obtained Fermi surfaces for a typical doping rate, $\delta = 0.139$, are shown in the insets of figure 3. As seen in figures 3(a) and (b), the angular dependence in the two hole-doped cases becomes concave for small $\phi$, namely near the nodal point, in contrast to the linear behavior of the simple $d_{x^2-y^2}$-wave symmetry indicated by the dotted lines. These deformations are significant especially for the regime near half-filling ($\delta \rightarrow 0$). This behavior is qualitatively consistent with experimentally observed angular dependences in Bi2212 [13, 14].

Next, let us discuss the electron-doped case. As shown in figure 2(c), the longer-range gap parameters are again meaningful. In this case, however, $\Delta_0^{(2)}$ is relatively small, but $\Delta_0^{(3)}(<0)$ has an appreciable absolute value of $0.1-0.2$. This long-range component deforms obviously the simple $d_{x^2-y^2}$-wave gap function. In figure 3(c), the resultant angular dependence of $\Delta_{\mathbf{k}}^{\text{ext.d}}$ in this case is shown for several values of $\delta$. In particular, for $\delta \leq 0.139$, the maxima are not located near the antinodal point, $\phi = \pi/4$, but in the middle of the nodal and antinodal points: $\pi/8 \lesssim \phi \lesssim 3\pi/16$. We find that these maximum positions are always close to the hot spots, i.e. the intersections of the Fermi surface with the AF magnetic Brillouin zone boundary. The vertical arrows in figure 3(c) indicate the hot-spot positions obtained from the Fermi surface of the optimized band $\tilde{E}_\mathbf{k}$ shown in the insets. Apparently, the hot spots are close to the maximum positions, although not exactly identical. This nonmonotonic behavior of $\Delta_{\mathbf{k}}^{\text{ext.d}}$ for the electron-doped case is consistent with the excitation gap deduced from experiments [15, 16]. Some theoretical studies have also discussed the nonmonotonic behavior of $\Delta_{\mathbf{k}}^{\text{ext.d}}$ in the electron-doped cases [37, 38]. They showed that the position of maximum $\Delta_{\mathbf{k}}^{\text{ext.d}}$ almost coincides with a hot spot.

The different behavior of $\Delta_{\mathbf{k}}^{\text{ext.d}}$ between the hole- and electron-doped cases will be understood from the difference of AF correlation. In the electron-doped case of the present model, equation (1), AF correlation is dominant owing to the nesting condition [39, 40]. As a result, $\Delta_0^{(2)}$ is suppressed while $\Delta_0^{(3)}$ is enhanced because parallel spin configurations are encouraged in the $(2, 0)$-position, while antiparallel configurations are favored in the $(3, 0)$-position. This tendency is apparent if we check the real-space spin correlation function, $\langle S_i^z S_j^z \rangle$, as shown in figure 4. In the electron-doped case, the AF correlation is dominant and $\langle S_i^z S_j^z \rangle$ has alternating signs until the correlation length of about six lattice constants. In contrast, the AF correlation in the hole-doped case is much weaker than in the electron-doped case. This is consistent with the above result that not only $\Delta_0^{(2)}$ but also the longer-range $\Delta_0^{(n)}$ have finite values in the hole-doped cases.

As mentioned in section 1, the optimized singlet gap parameter $\Delta_{\mathbf{k}}^{\text{ext.d}}$ represents the excitation gap of spinons without coherence of holons, but generally not a SC gap in the sense of slave-boson mean-field theory. Actually, $\Delta_{\mathbf{k}}^{\text{ext.d}}$ has finite values even at half-filling ($\delta = 0$) where a Mott insulator is realized. Hence, as a quantity representing the SC, we calculate a
Figure 3. Angular ($\phi$) dependence of optimized $\Delta_k^{\text{ext.d}}$ along the Fermi surface for various values of the doping concentration, $\delta$, for the three parameter sets: (a) $t'/t = -0.10$ and $t''/t = 0.10$ of LSCO, (b) $t'/t = -0.16$ and $t''/t = 0.20$ of YBCO and (c) $t'/t = 0.16$ and $t''/t = -0.20$ of NCCO. The numbers attached to the lines indicate the value of $\delta$. Here, the Fermi surface is determined from the optimized band, $\tilde{\epsilon}_k$, with band renormalization of $\tilde{t}'/t$ and $\tilde{t}''/t$. The obtained Fermi surfaces for a typical doping rate ($\delta = 0.139$) are shown in the insets, and the hot spots are also indicated by open circles. Note that the Fermi surface in (c) is of electrons and not of holes. In (c), the vertical arrows indicate the hot-spot positions for the corresponding doping rate, $\delta$. Dotted lines in (a)–(c) indicate the angular-dependences of the simple $d_{x^2-y^2}$-wave symmetry obtained using some $\Delta_0^{(1)}$. The data obtained in the system sizes of $L = 12$ and 14 are compared.
Figure 4. Real space spin correlation function, $\langle S^z_i S^z_j \rangle$, in a typical hole-doped case with $t'/t = -0.16$, $t''/t = 0.20$ and $\delta = 0.139$ (solid line), and in an electron-doped case with $t'/t = 0.16$, $t''/t = -0.20$ and $\delta = 0.139$ (broken line). Note that they are obtained in the extended $d_{x^2-y^2}$-wave BCS state, of equation (2). The system size is $L = 12$.

The long-distance value of SC correlation function:

$$P(\tau) = \frac{1}{N_S} \sum_i \left| \langle \Delta_\tau^x(R_i) \Delta_\tau(R_i + \mathbf{r}_M) \rangle \right|,$$

where $\Delta_\tau^x(R_i) = (c_{i\uparrow}^\dagger c_{i+\tau\uparrow}^\dagger + c_{i+\tau\downarrow}^\dagger c_{i\downarrow}^\dagger) / \sqrt{2}$, $\tau$ is the length of the pair, and $\mathbf{r}_M = (L/2, L/2)$ is the longest distance the pair can jump. In figure 5, $P(\tau)$'s for various pair length are shown as a function of $\delta$ for the three parameter sets. First, one can notice a marked asymmetry between the hole-doped cases (figures 5(a) and (b)) and the electron-doped case (figure 5(c)). $P(1)$ of the hole-doped case is considerably large and extended, compared to that of the electron-doped case. Furthermore, among the hole-doped cases, $P(1)$ is considerably larger and extended for the case of $t'/t = -0.16$ and $t''/t = 0.20$ (YBCO) than that for the case of $t'/t = -0.10$ and $t''/t = 0.10$ (LSCO). From figure 5, one can also see that $P(\tau)$'s for $\tau \geq 2$ are almost zero both for hole- and electron-doped cases, namely, the SC correlation is dominant only in the nearest neighbor pairing even though the singlet gap parameter, $\Delta_{k_{ext}}$, has contributions from farther sites. Therefore, the Fourier transform of $P(\tau)$ looks just as the simple $d_{x^2-y^2}$-wave symmetry.

4. Summary and discussions

To elucidate the origin of the gaps found in the high-$T_c$ cuprates, we evaluated the momentum dependence of the singlet gap parameter, $\Delta_{k_{ext}}$, and the SC correlation functions both with the $d_{x^2-y^2}$-wave symmetry in the $t-t'-t''-J$ model using an optimization VMC method. For small doping ($\delta \lesssim 0.2$), the singlet gap is significantly deformed from the simple $d_{x^2-y^2}$-wave due to the contributions of the long-range pairings. In the hole-doped cases, the angular dependence along the Fermi surface becomes concave near the nodal direction, whereas in the
Figure 5. Long-distance values of the real-space SC correlation function, \( P(\tau) \), for various pair length \( \tau = 1, 2, 3, 4, \sqrt{5}, \sqrt{10} \) and \( \sqrt{13} \) as a function of \( \delta \) for three parameter sets: (a) \( t'/t = -0.10, t''/t = 0.10 \) of LSCO, (b) \( t'/t = -0.16 \) and \( t''/t = 0.20 \) of YBCO and (c) \( t'/t = 0.16 \) and \( t''/t = -0.20 \) of NCCO. The data obtained in the system sizes of \( L = 12 \) and 14 are plotted simultaneously.

In the electron-doped case, the maxima of the singlet gap are located in the middle of the nodal and antinodal directions. These angular dependences qualitatively coincide with those observed in some experiments both in hole- and electron-doped cuprates. On the other hand, the SC correlation function is dominant in the nearest-neighbor pairings. Fourier transform of this almost preserves the original simple \( d_{x^2-y^2} \)-wave form \( (\propto \cos k_x - \cos k_y) \).

The present results indicate that the excitation spectra observed experimentally can be naturally understood from the behavior of the singlet gap parameter, \( \Delta_{\text{ext}}^k \), in the \( t-t'-t''-J \) model. Since the gap parameters are included in the wave function of equation (2), they can be regarded as an excitation gap in the spin degrees of freedom (or spinons) in the sense of the slave-boson mean-field approximation [18]. Although the present VMC method cannot be applied to finite temperatures, let us speculate on the pseudo-gap behavior above \( T_c \) in view of the present results. In the slave-boson mean-field theory, the state above \( T_c \) (or pseudo-gap state) is regarded as a resonating valence bond (RVB) state with spinon pairing but without
Bose condensation of holons [18]. Therefore, we expect that the wave function is similar to equation (2) but without coherence of holons. In this case, the singlet excitation gap will be similar to $\Delta^\text{ext.d}_k$ in figure 3. Thus the pseudo-gap above $T_c$ can be understood from $\Delta^\text{ext.d}_k$ with some incoherence due to disordered holons. Actually the obtained doping-dependence of $\Delta^\text{ext.d}_k$ is consistent with that of the pseudo-gap in the hole-doped cases. However, note that the pseudo-gap behavior is not completely understood because the pseudo-gap seems to vanish in a sizable area near the nodal points called a ‘Fermi arc’. To pursue this phenomenon, other factors may have to be introduced, such as the charge inhomogeneity, etc [8].

As for the coherent SC gap, recent experiments suggest that it appears below $T_c$ inside the ‘Fermi arc’ region. It is tempting to assume that this coherent SC gap is caused by the SC correlation $P(\tau)$ discussed in the present VMC calculation. Actually, $P(\tau)$ represents the true SC correlation that involves charge degrees of freedom, while the gap parameter, $\Delta^\text{ext.d}_k$, represents the spinon RVB gap. In fact, due to the Gutzwiller projection, $P(\tau)$ in equation (6) vanishes at half-filling in which the Cooper pairs cannot have kinetic energy. In the Gutzwiller approximation [19, 41], one can show that $P(\tau)$ is proportional to $\delta$ for small values of $\delta$. In this sense, $P(\tau)$ is finite only when the holons (or charge degrees of freedom) are coherent, which anticipates a close relationship to the SC gap. It is to be noted that the behavior of $P(\tau)$ agrees with $v_\Delta$ discussed in the Hubbard model [11], which represents the anomalous velocity parallel to the Fermi surface at the nodal point. It was discussed that $v_\Delta$ is proportional to the spectral weight of the quasiparticle at the nodal point. This corresponds to the coherent motion of holons in the present $t-J$ model. The obtained doping-dependence of $P(\tau)$ in figure 5 is consistent with that for the coherent SC gap. It also agrees with the recent claim that the coherent gap correlates with $T_c$.

In summary, the doping dependence and angular dependence of $\Delta^\text{ext.d}_k$ and SC correlation function seem to be consistent with the pseudo-gap and the coherent SC gap inside the ‘Fermi arc’. However, in order to establish these correspondences, it is still necessary to investigate these quantities in other methods.

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New Journal of Physics 11 (2009) 075011 (http://www.njp.org/)
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New Journal of Physics 11 (2009) 075011 (http://www.njp.org/)