Phenomenological model for two gap states in underdoped high-temperature superconductors and short-range antiferromagnetic correlation effect

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Assuming antiferromagnetic orbital correlations to model the pseudogap state in the underdoped high-temperature superconductors, we study how this correlation is distinguished from the d-wave superconductivity correlation with including the finite-range antiferromagnetic correlation effect. In spite of the fact that both correlations have the same d-wave symmetry, the contributions from each correlation is clearly distinguished in the spectral weight and the density of states.

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In the high-temperature superconductors, the origin of the pseudogap state is still in controversial. Contrary to conventional superconductors, behaviors associated with opening some gap are observed in various experiments above the transition temperature to the superconducting state, \( T_c \). Concerning the origin of the pseudogap, mainly there are two pictures. One is to assume that the pseudogap is associated with precursor of superconductivity. The other is to assume another gap formation which is different from the superconducting gap.

Recent angle-resolved photoemission spectroscopy measurements seem to support two gap scenario. In the normal state, the full Fermi surface is clearly observed. Along this Fermi surface, the gap has been measured in the superconducting state. Around the nodal region, the gap is well fitted by a d-wave superconducting gap. As moving away from the node, the gap deviates from the line expected from the simple d-wave superconducting gap. The doping dependence of the gap around the node is increased in the underdoped regime. By contrast, the gap around the antinodal region decreases. Furthermore, the gap around the antinode shows negligible change across \( T_c \) whereas the gap around the node shows significant variation. This result suggests that those gaps have different origins. This is consistent with the recent Raman scattering experiments.

In the Raman scattering experiments the nodal region and the antinodal region are distinguished by symmetry. From \( B_{1g} \) and \( B_{2g} \) spectra, the Raman shifts show qualitatively different behaviors. The shift associated with the node (\( B_{2g} \)) increases as the doping concentration is increased while the shift associated with the antinode (\( B_{1g} \)) decreases.

The two gap picture is also supported by scanning tunneling microscopy (STM). About a decade ago, some STM measurements supported that the pseudogap and the superconducting gap had the same origin because the pseudogap seemed to smoothly evolve into the superconducting gap as decreasing temperature. However, in the recent STM measurements it is found that there are two components: One is inhomogeneous and the other is homogeneous. The inhomogeneous component is associated with relatively high-energy features and it is found that that component does not show clear temperature dependence around \( T_c \). By contrast, the inhomogeneous component does not show qualitative difference at \( T_c \). It is also found that the gap value estimated for the homogeneous component is reduced from that estimated from the raw data. It is known that the latter gap \( \Delta_o \) is scaled by the pseudogap temperature, \( T^* \), with \( 2\Delta_o \approx 4.3k_BT^* \). This scaling relation is consistent with the orbital antiferromagnetic correlation with d-wave symmetry.

If both of superconductivity and the pseudogap are characterized by d-wave symmetry, then the question is how we can distinguish these correlations in the physical quantities. To answer this question, we study a simple phenomenological model for the two gap state for high-temperature superconductors. We assume the d-wave BCS gap for superconductivity and d-wave orbital antiferromagnetic correlation to model the pseudogap. Based on this model we compute the spectral weight along the underlying Fermi surface and the density of states with including the short-range antiferromagnetic correlation effect. In spite of the fact that the two gaps have the same symmetry, we find that these components are clearly distinguished in the Brillouin zone and in the density of states.

The model Hamiltonian is given by
\[
H = \sum_{k \in RBZ} \left( c_{k\uparrow}^\dagger c_{-k\downarrow} + c_{-k+Q\uparrow}^\dagger c_{-k-Q\downarrow}^\dagger \right) \begin{pmatrix} \varepsilon_k - \mu & \Delta_{k}^{SC} & i\Delta_k & 0 \\ \Delta_{k}^{SC} & -\varepsilon_k + \mu & 0 & i\Delta_k \\ -i\Delta_k & 0 & -\Delta_{k}^{SC} & -\varepsilon_k + Q - \mu \\ 0 & -i\Delta_k & -\Delta_{k}^{SC} & \varepsilon_k + Q - \mu \end{pmatrix} \begin{pmatrix} c_k \varepsilon_k - \mu & + & (\varepsilon_k+Q - \mu) \end{pmatrix}.
\]

where \( \varepsilon_k = -2t_0 (\cos k_x + \cos k_y) - 4t_1 \cos 2k_x \cos k_y - 2t_2 (\cos 2k_x + \cos 2k_y) \), \( \Delta_k = \frac{\Delta_{Q}^{AF}}{2} (\cos k_x - \cos k_y) \), and \( \Delta_{Q}^{SC} = \frac{\Delta_{0}^{SC}}{2} (\cos k_x - \cos k_y) \). The summation with respect to \( k \) is taken over the reduced Brillouin zone, \(|k_x| < \pi \) and \(|k_y| < \pi \). The wave vector \( Q \) is fixed to \( Q = (\pi, \pi) \) for the pure mean field state. In order to include the short-range antiferromagnetic correlation effect approximately, we assume that \( Q \) obeys a Lorentzian probability distribution whose peak is at \( (\pi, \pi) \) with broadening factor of \( \xi_{AF} \). We follow the analysis described in Ref.\[15\] in investigating the short-range antiferromagnetic correlation effect.

The energy dispersions are obtained by diagonalizing \[1\],

\[
E_k^{(\pm, \pm)} = \pm \sqrt{\left( \varepsilon_k^{(+)} - \mu \right) \pm \sqrt{\left( \varepsilon_k^{(-)} \right)^{2} + \Delta_k^{2}}} + \left( \Delta_{k}^{SC} \right)^{2}.
\]

Here \( \varepsilon_k^{(+)} = \frac{\varepsilon_k + \varepsilon_{k} + Q}{2} \) and \( \varepsilon_k^{(-)} = \frac{\varepsilon_k - \varepsilon_{k} + Q}{2} \). For the calculation of the spectral weight, we compute the Matsubara Green’s function, \( G_{k\uparrow} (\tau) = - \left\langle T_{\tau} c_{k\uparrow}^\dagger \tau \right\rangle c_{k\uparrow} (0) \). Transforming to the Matsubara frequency from the imaginary time \( \tau \), we have

\[
G_{k\uparrow} (i\omega_n) = \sum_{\alpha} \frac{4}{U_{k\uparrow,\alpha}} \frac{U_{k\uparrow,\alpha} (U_{\uparrow})^\dagger_{\alpha,k\downarrow}}{i\omega_n - E_n}.
\]

The Unitary matrix \( U_{k\uparrow,\alpha} \) is computed numerically diagonalizing Eq. \[1\]. The index \( \alpha \) is for the energy bands. We have four bands for \( \Delta_0^{SC} \neq 0 \) and \( \Delta_0 \neq 0 \).

In Fig.\[1\] the spectral weight at the Fermi energy is shown. The solid line represents the underlying Fermi surface which is given by \( \varepsilon_k = \mu \). The chemical potential \( \mu \) is determined from

\[
x = 1 - \frac{1}{2N_s} \sum_k n_k,
\]

with \( n_k = 2 + \left\langle c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger \right\rangle - \left\langle c_{-k\downarrow}^\dagger c_{-k\uparrow}^\dagger \right\rangle + \left\langle c_{k+Q\uparrow}^\dagger c_{k+Q\downarrow}^\dagger \right\rangle - \left\langle c_{-k-Q\downarrow}^\dagger c_{-k-Q\uparrow}^\dagger \right\rangle, \ x \) the doped hole concentration and \( N_s \) the number of the lattice sites. The expectation values are calculated by diagonalizing \[1\]. We take the hopping parameters as \( t_0 = 1 \), \( t_1 = -0.25 \), and \( t_2 = 0.10 \) throughout the paper.

![Figure 1: Spectral weight at the Fermi energy averaged over probability distribution with respect to \( Q \). The antiferromagnetic correlation length is \( \xi_{AF} = 4 \). The solid line represents the underlying Fermi surface with \( \Delta_0^{SC} = 0 \) and \( \Delta_0 = 0 \).](image)

Although we assume a finite antiferromagnetic correlation length, the mean field calculation shows that \( 2\Delta_0/k_BT^* \approx 4.8 \) for the interaction \( V = 2 \) and \( \xi_{AF} = 4 \) on \( 50 \times 50 \) lattice. Therefore, we may assume a finite value of \( \Delta_0 \) in spite of the lack of the orbital antiferromagnetic long range ordering.

Figure\[2\] shows the spectral weight along the Fermi surface at fixed \( Q = (\pi, \pi) \). In order to identify the contributions from the superconductivity correlation and the orbital antiferromagnetic correlation, we compare the result with or without each correlation. One can see that the structure around the superconducting gap node is mainly determined by the d-wave superconductivity correlation. Meanwhile the antinode structure is mainly determined by the orbital antiferromagnetic correlation.

Figure\[3\] shows the dispersion energies along the underlying Fermi surface. By comparing with Fig\[2\] we see that a part of the energy dispersions is invisible in the spectral weight because of the coherence factor effect. As shown in Fig.\[4\] the energy dispersion around the node is well described by d-wave gap function. Around the antinode, the energy dispersion is also well described by d-wave symmetry. However, this component is dominated
by the orbital antiferromagnetic correlation as suggested from Fig. 2. This analysis suggests that clear information about the superconducting gap is extracted near the node. In fact, from the linear function fitting of the gap near the node we find $\Delta_{SC}$ from Fig. 4. By contrast, the gap near the antinode contain both contributions of the superconductivity correlation and the orbital antiferromagnetic correlation. It is hard to decompose these components even in our idealized model.

Next we compute the density of states as follows

$$D(\omega) = \sum_k \sum_{\alpha=1}^4 \delta \left( \omega - E_k^{(\alpha)} \right).$$

For numerical computations, we replace the delta function with a Lorentzian. The broadening factor is chosen as 0.10. In Fig. 5 we show $D(\omega)$ for different values of $\xi_{AF}$. We can distinguish each band contribution. The peaks around $\omega \approx \pm 1$ are associated with the orbital antiferromagnetic correlation. While the shoulders around $\omega \approx \pm 0.3$ are associated with the superconductivity correlation. These features become sharp for large $\xi_{AF}$. But the broadening effect due to $Q$ fluctuations are similar as shown in Fig. 6. This result suggests that inhomogeneity of the relatively high energy component is not associated with the antiferromagnetic correlation effect.

Figure 7 shows the intersection of $D(\omega)$ at $\omega = 0.079$. The same result is obtained at $\omega = -0.079$. For large $\xi_{AF}$, we see some weight outside of the reduced Brillouin zone. By contrast, this weight disappears for short $\xi_{AF}$. As a result, we see a banana shape as seen in STM experiments.

To summarize, we study the spectral weight and the density of states in the presence of both of d-wave superconductivity correlation as suggested from Fig. 2. This analysis suggests that clear information about the superconducting gap is extracted near the node. In fact, from the linear function fitting of the gap near the node we find $\Delta_{SC}$ from Fig. 4. By contrast, the gap near the antinode contain both contributions of the superconductivity correlation and the orbital antiferromagnetic correlation. It is hard to decompose these components even in our idealized model.
perconductivity correlation and the orbital antiferromagnetic correlation with taking into account the finite-range of the antiferromagnetic correlation effect. Although these correlations are assumed to have the same \( \hat{d} \)-wave symmetry, it is demonstrated that these components are clearly distinguished in the spectral weight and the density of states. As for asymmetry of the density of states, we need to include impurity scattering effect as demonstrated in Ref. [16].

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