Spectral Weights, $d$-wave Pairing Amplitudes, and Particle-hole Tunneling Asymmetry of a Strongly Correlated Superconductor

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The emergence of the superconductivity as holes doped into the Mott insulating parent compounds is one of the intriguing phenomena of high $T_c$ cuprates. It is usually emphasized, however, below the transition temperature there is strong similarity of the superconducting (SC) state with that of low $T_c$ for removing an electron and thin superfluid density (SC) state with that of low $T_c$ cuprates. Nevertheless, differences from the conventional SC state are unearthed clearly by high-resolution scanning tunneling microscopy and spectroscopy (STM/STS) on different cuprates with easily-cleaved surfaces. Namely, despite of physical quantities with nanometer scale inhomogeneity, the averaged (over some area within the scanned field-of-view) tunneling conductance is of unexpected behavior: its amplitude at negative sample bias - for removing electrons - is often larger than that at positive one - for adding electrons. Most intriguingly, the gap size, which was usually inferred from photoemission experiments, can be extracted directly from conductance peaks for the first time and is found to be larger as peaks become less pronounced. Same behaviors have been observed previously in underdoped cuprates using point-contact tunneling set-up.

The theoretical attempt to understand the features seen in STM/STS hit hitherto is mostly about the effects of the inhomogeneous dopant induced SC order parameters to the local density of states (LDOS) of the $d$-wave BCS ($d$-BCS) state, it largely neglects the strong correlation between electrons which should be essential for the case of underdoped cuprates. Actually, there is not enough understanding about the effect of strong correlation for a homogeneous system to help us to address the complex issues of disorder as revealed by tunneling experiments. Recently, Anderson proposed that the asymmetric tunneling conductance is closely related to the strong correlations inherent in the Gutzwiller projected $d$-BCS or, simply, resonating-valence-bond wave function (RVB WF). However, treating the projection only approximately by the usual scheme of the renormalized mean-field theory (RMFT), there have been controversy whether the asymmetry is accounted for by the coherent quasi-hole (QH) and -particle (QP) excitations of the projected state or rather by the incoherent part dictated by the spectral sum rule. Also, the correlation between gap sizes and peak heights has not yet been examined clearly from the strong correlation point of view.

In this paper, we defer the issue of inhomogeneity to later work and examine exactly the effects of strong correlation by numerically investigating the spectral weights (SW's) of the $d$-wave RVB ($d$-RVB) state on finite square lattices. With SW, particularly, $Z_{k\sigma}$ for removing an electron (defined in Eq. (1) below), calculated, we obtained several results: (i) $d$-wave pairing amplitude squared is equal to the products of SW's as it is exactly for weakly-coupled case; (ii) inspired by the hole doped case we focus mostly here, a rigorous relation of the heights of SW peaks decrease as the gap sizes increase. Same behaviors have been observed previously in underdoped cuprates using point-contact tunneling set-up.

Let us start by defining the SW for adding (and removing) one electron we calculate, i.e.

$$Z_{k\sigma}^{(+)} = \frac{\langle N_e + (-1) \mid c_{k\sigma} \mid N_e \rangle}{\langle N_e \mid N_e \rangle \langle N_e + (-1) \mid N_e + (-1) \rangle},$$

(1)

where, for momentum $k$,

$$\mid N_e + 1 \rangle \equiv P_d \mid c_{k\sigma} \mid N_e \rangle_0$$

(2)
for the QP excitation, and

$$\left| N_c - 1 \right\rangle \equiv P_d e^{i\vec{k} \cdot \vec{\sigma}} \left| N_c - 2 \right\rangle_0$$ \hspace{1cm} (3)

for the QH one which is also proportional to $P_d e^{i\vec{k} \cdot \vec{\sigma}} \left| N_c \right\rangle_0$. Here $\left| N_c \right\rangle_0$ is related to the trial WF of the projected electron-paired ground state in a uniform system,

$$\left| N_c \right\rangle = P_d \left| N_c \right\rangle \equiv P_d \left( \sum_q a^+_q c^+_q \right)^{N_c/2}$$ \hspace{1cm} (4)

The variationally optimized $\left| N_c \right\rangle$ we focus on in this paper is the $d$-RVB state. With $N_c$ the total number of electrons, coefficient $a_q = n_q/u_q = (E_q - \epsilon_q)/\Delta_q$ in which $n_q$ and $u_q$ are SC coherent factors, $\epsilon_q = -(\cos q_x + \cos q_y) - \mu - t' \cos q_x \cos q_y - t''(\cos 2q_x + \cos 2q_y)$, $\Delta_q = \Delta_v (\cos q_x - \cos q_y)$, and $E_q = \sqrt{\epsilon^2_q + \Delta^2_q}$. The operator $P_d$ projects out the doubly-occupied sites in the system with a finite number of doped holes present. In addition to $\Delta_v$, $\mu$, $t'$, $t''$ are the other two variational parameters associated with the long-range hoppings in the $t$-$t'$-$t''$-$J$ model Hamiltonian, $H = -\sum_{i,j} P_d t_{ij} (c^\dagger_i \sigma c_{j,\sigma} + h.c.) P_d + J \sum_{<i,j>} \langle \hat{S}_i \cdot \hat{S}_j - 1/4 n_i n_j \rangle$, where hopping amplitude $t_{ij} = t'$, and $t''$ for sites $i$ and $j$ being the nearest-, next-nearest-, and the third-nearest-neighbors, respectively. $\hat{S}_i$ the spin operator at site $i$, $i < i, j >$ means that the interaction between spins occurs only for the nearest-neighboring sites.

Applying identities for projection operator,

$$[c^\dagger_{k,\sigma}, P_d] P_d = 0; \hspace{1cm} P_d c^\dagger_{k,\sigma} c_{k',\sigma} P_d = P_d \left( \frac{1}{N} \sum_i e^{i(k' \cdot \vec{r}_i)} \hat{R}_{i,\sigma} n_{i,-\sigma} \right) P_d$$ \hspace{1cm} (5)

with $\hat{R}_{i,\sigma}$ the position vector of the $i$-th spin $\sigma$ in the lattice of size $N$ and $n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$, we can relate the $Z_{k,\sigma}^+$ exactly to the momentum distribution function (MDF) $n_{k,\sigma}$ as

$$Z_{k,\sigma}^+ = \frac{1 + x}{2} - n_{k,\sigma},$$ \hspace{1cm} (6)

where $x$ is the density of doped holes and $n_k = \langle N_c | c^\dagger_{k,\sigma} c_{k,\sigma} | N_c \rangle / \langle N_c | N_c \rangle$.

As a digression to electron doped (ED) case, it is straightforward to show that, applying the hole-particle transformation to Fig. 4, the SW of removing an electron in ED system satisfies rigorously $Z_{k,\sigma} = n_{k,\sigma} - (1 - x)/2$. This relation may be verified in experiment.

Back to the hole doped case, although there is no exact relation like this for $Z_{k,\sigma}^-$, we notice that $Z_{k,\sigma}^-$ and $Z_{k,\sigma}^+$ satisfy a relation,

$$Z_{k,\sigma}^- \cdot Z_{k,\sigma}^+ = \left( \frac{\langle N_c | c^\dagger_{k,\sigma} c_{k,\sigma} | N_c - 2 \rangle}{\langle N_c | N_c \rangle \langle N_c - 2 | N_c - 2 \rangle} \right)^2 \equiv P_k$$ \hspace{1cm} (7)

which can be proved straightforwardly by combining Eqs. (5) and (6). The matrix element $\hat{R}_k$, which represents the off-diagonal long-range order in the pairing correlation, is related to the $d$-wave SC pairing amplitude or order parameter $\Delta_{op}$ by

$$\Delta_{op} = \frac{2}{N} \sum_k \langle \cos k_x - \cos k_y \rangle \sqrt{P_k}.$$ \hspace{1cm} (8)

With both the SW’s computed numerically, we plot in Fig. 1 the doping dependence of $\Delta_{op}$ which indeed has the dome-like shape similar to the $T_c$ versus doping determined experimentally. Actually, the peak positions shown in Fig. 4 are almost the same as what have been obtained previously by studying the $d$-wave long-range pair-pair correlation. With more holes doped into the system, just like the reduction of long-range correlation between electron pairs is induced by the change of the anti-nodal Fermi surface geometry, the SC order parameter is decreased due to $Z_{k,\sigma}$ with $k$ near $(\pi, 0)$. Hence Eq. (7) provides another way to evaluate the strength of the pairing amplitude.

For the BCS theory without projection, we know $Z_{k,\sigma}^\pm = u_{k,\sigma}^2 (v_{k,\sigma}^2)$ and Eq. (8) is also exactly satisfied. For the strongly correlated $t$-$J$-type models, even though the same relation is followed in RMFT, it is still surprising to find out that this relation is correct in the RVB state with projection rigorously obeyed.

On the other hand, reminiscent of what have been argued previously by analytic approach, we recognize that the strong correlation effects becomes apparent only in $Z_{k,\sigma}$ at low doping. The effects due to strong correlation are examined by comparing the coherent SW’s averaged over all momenta, i.e. $Z_{ave} \equiv \sum_k Z_{k,\sigma}/N$, and the incoherent part defined by the relation

$$n_{ave} \equiv n_{ave} - Z_{ave}$$ \hspace{1cm} (9)

obtained by exact treatment of the projection and by using RMFT. Here $n_{ave} \equiv \sum_k n_{k,\sigma}/N$ is the average MDF.

![FIG. 1: The SC pairing amplitude for d-RVB state as a function of doping determined by the products of SW’s using Eqs. 4 and 5. System size here is 12x12. Different symbols represent results obtained for different values of $(t', t'')/t$, as indicated.](image-url)
which should always be equal to the electron density of the system.

The exact results for the 12 × 12 lattice and that by RMFT are shown in Fig. 2. The coherent part of $Z_{k\sigma}^-$ by RMFT is $g_k t^2 \sigma$ with renormalization factor $g_k = 2x/(1+x)$. Completing the momentum sum for the coherence factor, the average result is $x(1-x)/(1+x)$ and, thus, $n_{ave} = [(1-x)^2]/2(1+x)$, plotted in Fig. 2 (dashed and dotted lines, respectively) in comparison with the exact ones. As is shown there, while the numerical $n_{ave}$ (solid circles) is indeed equal to the electron density, the exact incoherent SW for removing an electron is less than the RMFT result. The difference becomes more significant as hole doping level is reduced. Interestingly, this behavior is independent of the $(t', t'')/t$ values (represented by solid and empty symbols in Fig. 2) which correspond to very different doping dependence of the Fermi surface shape and also the DOS. By contrast, the average values of $Z_{k\sigma}^+$ calculated exactly (not shown) and by RMFT are identical due to Eq. (4).

To make a comparison with tunneling experiments, we then concentrate on the SW’s as a function of the excited-state energy. By applying the model Hamiltonian to excitations $|N, \pm 1\rangle$, we calculate their excitation energies for each momentum and also the corresponding energy gap by fitting the excitation energy $E_k$. To reduce the effect of finite size, we define the sum of $Z_{k\sigma}^+ / N$, over momentum $k$ which has energy within $E - \Delta E / 2$ and $E + \Delta E / 2$, as $g(E)$ [negative (positive) for removing (adding) an electron] which could be viewed, approximately, as proportional to the conductance at low energy $E$. We plot $g(E)$ in Fig. 3 up to about the energy where peaks appear for lattices of size 12 × 12 with $\Delta E / t = 0.3$, and also 20 × 20 with energy interval 0.2 for various dopings.

To make sure our treatment is correct, we have also applied the same analysis to the d-BCS state. As shown in the inset of Fig. 3, the ideal BCS result is hardly distorted by the finite size. Note that, with the reasonable finite-size dependence, we obtain indeed the V-shape $d$-wave gap near zero energy. The width between peak positions is also roughly equal to two times of the gap value deduced from the excitation energy. Looking at the results closely, while $g(E)$ may indeed be about the same at the opposite sides in the very vicinity of zero energy as suggested in Ref.22, $g(E)$ for removing an electron is always larger than that for adding an electron at higher energy near that of the peak. With decreased doping, the ratio of $g(E)$ at negative and positive energies enhances quite dramatically, e.g. from $x = 0.125$ to 0.056, $g(-\Delta) / g(\Delta)$ at the corresponding energy of the peak $\Delta$ (in units of $t$) increases from 1.96 to 2.73. Similar behaviors are found for the case with vanishing $(t', t'')/t$ (not shown). In contrast to this, for the d-BCS (inset in Fig. 3) case in the same finite lattices there is almost no change of the ratio within the gap. The numerical results thus tells us features due to strong correlation which are not fully explored yet in the tunneling experiment, i.e. the particle-hole asymmetry of average conductance exists even within the gap region and gets enhanced with underdoping.

Fig. 3 also reveals correlation between heights of the spectral weight peak and the gap size (or the width between peaks) as doping level is varied. Within the doping level shown in Fig. 3, the peak height scales with the pairing amplitude but apparently anti-correlates with the gap size. This is in clear contrast to the BCS case in which the peak height, proportional to the SC coher-
ence, scales with the width between peaks or gap size as more holes doped into the system. Our result agrees qualitatively with what has been extracted from STS experiments.

To conclude, in order to provide a better understanding of the results measured by the tunneling experiments without the complication of mixing disorder and strong correlation, here we studied the SW’s for adding and removing an electron for a uniform d-RVB SC state without disorder. We derive analytically and examine numerically the relation between pairing amplitude and SW products. Performing particle-hole transformation, we obtain also exact dependence of SW for removing an electron with doping in the ED systems, which could be tested by photoemission spectroscopy. While the strong correlation effect is less noticeable by looking at the pairing amplitude, we found that the SW for removing an electron deviates clearly from results obtained by RMFT in the low doping regime. More specifically, at this doping level the conductance-related quantity of the uniform d-RVB state on finite lattices computed exactly is particle-hole asymmetric below the gap energy and, consistent qualitatively with what is seen in recent tunneling experiments, the extracted gap value (from the excitation energy) or, equivalently, the width between SW peaks anti-correlates with the peak heights.

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