Spectral weights, *d*-wave pairing amplitudes, and particle-hole tunneling asymmetry of a strongly correlated superconductor

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The spectral weights (SW's) for adding and removing an electron of the Gutzwiller projected *d*-wave superconducting (SC) state of the *t*-*J*-type models are studied numerically on finite lattices. We restrict the study to the uniform system but exactly treat the strong correlation between electrons, we show that the product of weights is equal to the pairing amplitude squared, the same as in the weakly coupled case. In addition, we derive a rigorous relation of SW with doping in the electron doped system and obtain particle-hole asymmetry of the conductance-proportional quantity within the SC gap energy and, also, the anticorrelation between gap sizes and peak heights observed in tunneling spectroscopy on high T_c cuprates.

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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.[1] It is usually emphasized, however, that below the transition temperature there is a strong similarity of the superconducting (SC) state with that of low T_c materials in the sense that the state is composed of Cooper pairs of electrons, though with unconventional *d*-wave pairing symmetry[2] and thin superfluid density.[3] 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 the physical quantities with nanometer scale inhomogeneity, the averaged (over some area within the scanned field-of-view) tunneling conductance is of an unexpected behavior: its amplitude at negative sample bias—*for removing electrons*—is often larger than that at the positive one—*for adding electrons*.[4–7] Most intriguingly, the gap size, which was usually inferred from photoemission experiments,[8] can be extracted directly from conductance peaks for the first time and is found to be larger as peaks become less pronounced.[5–7] The same behaviors have been observed previously in underdoped cuprates using a point-contact tunneling setup.[9]

The theoretical attempt to understand the features seen in STM/STS *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,[10] it largely neglects the strong correlation between electrons which should be essential for the case of underdoped cuprates.[11] 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).[12] However, treating the projection only approximately by the usual scheme of the renormalized mean-field theory (RMFT), there has been controversy as to whether the asymmetry is accounted for by the coherent quasihole (QH) and -particle (QP) excitations of the projected state or rather by the incoherent part dictated by the spectral sum rule.[13–15] Also, the correlation between gap sizes and peak heights has not yet been examined clearly from the strong correlation point of view.[16]

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, $Z_{\mathbf{k}\sigma}^{-}$ 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 the weakly-coupled case; (ii) inspired by the hole doped case we focus mostly on here, a rigorous relation of SW for removing an electron is derived for the electron doped case; (iii) the difference between $Z_{\mathbf{k}\sigma}^{-}$ calculated exactly and by using RMFT becomes significant at low, finite doping of holes; (iv) the particle-hole asymmetry of the sum of low-energy SW's over momenta within some energy window near the Fermi level becomes more prominent with reduced doping[17] and, meanwhile, (v) the heights of SW peaks decrease as the gap sizes increase.

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

$$Z_{\mathbf{k}\sigma}^{+(-)} = \frac{|\langle N_e + (-)1|c_{\mathbf{k}\sigma}^{\dagger}(c_{\mathbf{k}\sigma})|N_e\rangle|^2}{\langle N_e|N_e\rangle\langle N_e + (-)1|N_e + (-)1\rangle}, \tag{1}$$

where, for momentum $\mathbf{k}$,

$$|N_e + 1\rangle \equiv P_d c_{\mathbf{k}\sigma}^{\dagger}|N_e\rangle_0 \tag{2}$$

for the QP excitation, and

$$|N_e - 1\rangle \equiv P_d c_{-\mathbf{k}-\sigma}^{\dagger}|N_e - 2\rangle_0 \tag{3}$$

for the QH one which is also proportional to $P_d c_{\mathbf{k}\sigma}|N_e\rangle_0$. Here $|N_e\rangle_0$ is related to the trial WF of the projected electron-paired ground state in a uniform system,

$$|N_e\rangle = P_d|N_e\rangle_0 \equiv P_d\left(\sum_{\mathbf{q}} a_{\mathbf{q}} c^{\dagger}_{\mathbf{q}\uparrow} c^{\dagger}_{-\mathbf{q}\downarrow}\right)^{N_e/2}|0\rangle. \quad (4)$$

The variationally optimized $|N_e\rangle$ we focus on in this paper is the d-RVB state.[18] With N_e the total number of electrons, coefficient $a_{\mathbf{q}}=v_{\mathbf{q}}/u_{\mathbf{q}}=(E_{\mathbf{q}}-\epsilon_{\mathbf{q}})/\Delta_{\mathbf{q}}$ in which $v_{\mathbf{q}}$ and $u_{\mathbf{q}}$ are SC coherent factors, $\epsilon_{\mathbf{q}}=-(\cos q_x+\cos q_y)-\mu-t'_v\cos q_x\cos q_y-t''_v(\cos 2q_x+\cos 2q_y)$, $\Delta_{\mathbf{q}}=\Delta_v(\cos q_x-\cos q_y)$, and $E_{\mathbf{q}}=\sqrt{\epsilon_{\mathbf{q}}^2+\Delta_{\mathbf{q}}^2}$. The operator P_d projects out the doubly occupied sites in the system with a finite number of doped holes present. In addition to Δ_v and μ, t'_v and t''_v are the other two variational parameters associated with the long-range hoppings in the t-t'-t''-J model Hamiltonian, $H=-\Sigma_{ij}P_d t_{ij}(c^{\dagger}_{i,\sigma}c_{j,\sigma}+\mathrm{H.c.})P_d+J\Sigma_{<i,j>}\left(\vec{S}_i\cdot\vec{S}_j-\frac{1}{4}n_i n_j\right)$, where hopping amplitude $t_{ij}=t$, t', and t'' for sites i and j being the nearest-, next-nearest-, and the third-nearest-neighbors, respectively, $\vec{S}_i$ the spin operator at site i, $\langle i,j\rangle$ means that the interaction between spins occurs only for the nearest-neighboring sites.

Applying identities for the projection operator,

$$[c_{\mathbf{k}\sigma},P_d]P_d=0;$$

$$P_d c_{\mathbf{k}\sigma}[c^{\dagger}_{\mathbf{k}'\sigma},P_d]=P_d\left[\frac{1}{N}\sum_i e^{i(\mathbf{k}'-\mathbf{k})\cdot\vec{R}_{i\sigma}}n_{i,-\sigma}\right]P_d \quad (5)$$

with $\vec{R}_{i\sigma}$ the position vector of the ith spin σ in the lattice of size N and $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$, we can relate the $Z^{+}_{\mathbf{k}\sigma}$ exactly to the momentum distribution function (MDF) $n_{\mathbf{k}\sigma}$ as follows:

$$Z^{+}_{\mathbf{k}\sigma}=\frac{1+x}{2}-n_{\mathbf{k}\sigma}, \quad (6)$$

where x is the density of doped holes and $n_{\mathbf{k}}=\langle N_e|c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|N_e\rangle/\langle N_e|N_e\rangle$.[20–22]

As a digression to electron doped (ED) case, it is straightforward to show that, applying the hole-particle transformation to Eq. (6),[19] the SW of removing an electron in an ED system rigorously satisfies $Z^{-}_{\mathbf{k}\sigma}=n_{\mathbf{k}\sigma}-(1-x)/2$. This relation may be verified in experiment.

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

$$Z^{+}_{-\mathbf{k}-\sigma}\cdot Z^{-}_{\mathbf{k}\sigma}=\frac{|\langle N_e|c^{\dagger}_{\mathbf{k}\sigma}c^{\dagger}_{-\mathbf{k}-\sigma}|N_e-2\rangle|^2}{\langle N_e|N_e\rangle\langle N_e-2|N_e-2\rangle}\equiv P_{\mathbf{k}} \quad (7)$$

which can be proved straightforwardly by combining Eqs. (3) and (5). The matrix element $P_{\mathbf{k}}$, which represents the off-diagonal long-range order in the pairing correlation, is related to the d-wave SC pairing amplitude or order parameter Δ_{op} by

$$\Delta_{op}=\frac{2}{N}\sum_{\mathbf{k}}|\cos k_x-\cos k_y|\sqrt{P_{\mathbf{k}}}. \quad (8)$$

With both the SW's computed numerically, we plot in Fig. 1 the doping dependence of Δ_{op} which indeed has the *dome-like* shape similar to the T_c versus doping determined experimentally. Actually, the peak positions shown in Fig. 1 are almost the same as what have been obtained previously by studying the d-wave long-range pair-pair correlation.[18,23] Furthermore, 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 antinodal Fermi surface geometry,[18] the SC order parameter is decreased due to $Z^{-}_{\mathbf{k}\sigma}$ with $\mathbf{k}$ near $(\pi,0)$. Hence Eq. (7) provides another way to evaluate the strength of the pairing amplitude.

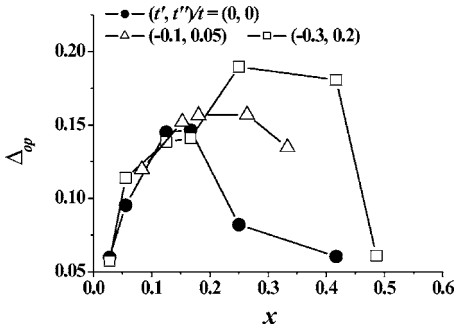

FIG. 1. The SC pairing amplitude for d-RVB state as a function of doping determined by the products of SW's using Eqs. (7) and (8). System size here is 12×12. Different symbols represent results obtained for different values of $(t',t'')/t$, as indicated

For the BCS theory without projection, we know $Z^{+(-)}_{\mathbf{k}\sigma}=u^2_{\mathbf{k}}(v^2_{\mathbf{k}})$ and Eq. (7) is also exactly satisfied. For the strongly correlated t-J-type models, even though the same relation is followed in RMFT (Ref. 24), it is still surprising to find out that this relation is correct in the RVB state with the projection rigorously obeyed.

On the other hand, reminiscent of what has been argued previously by analytic approach,[13] we recognize that the strong correlation effects becomes apparent only in $Z^{-}_{\mathbf{k}\sigma}$ at low doping. The effects due to strong correlation are examined by comparing the *coherent* SW's averaged over all momenta, i.e., $Z^{-}_{ave}\equiv\Sigma_{\mathbf{k}}Z^{-}_{\mathbf{k}\sigma}/N$, and the *incoherent* part defined by the relation

$$n^{inc}_{ave}\equiv n_{ave}-Z^{-}_{ave} \quad (9)$$

obtained by exact treatment of the projection and by using RMFT. Here $n_{ave}\equiv\Sigma_{\mathbf{k}}n_{\mathbf{k}\sigma}/N$ is the average MDF 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 $Z^{-}_{\mathbf{k}\sigma}$ by RMFT is $g_t v^2_{\mathbf{k}}$ with a renormalization factor $g_t=2x/(1+x)$. Completing the momentum sum for the coherence factor, the average result is $x(1-x)/(1+x)$ and, thus, $n^{inc}_{ave}=[(1-x)^2]/2(1+x)$,[14] 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 the 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

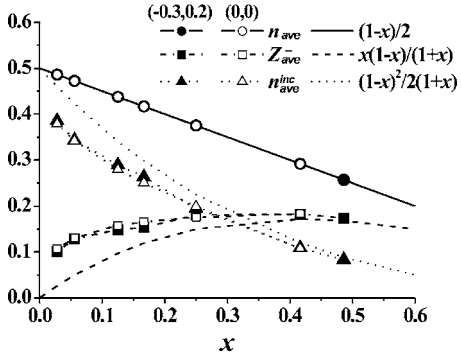

FIG. 2. The doping dependence of SW's for removing an electron and average MDF of d-RVB state obtained numerically for the 12×12 lattice and by RMFT. Numerical and expected n_{ave} are denoted by the circles and the solid line, respectively. The squares (triangles), connected by dashed (dotted) line as the guide for the eye, are for exact results of Z^{-}_{ave} [n^{inc}_{ave}, extracted using Eq. (9) with n_{ave} calculated numerically]. All solid symbols are results for $(t',t'')/t=(-0.3,0.2)$ and empty ones for (0,0). The dashed and dotted lines without data points represent results by RMFT.

of $Z^{+}_{\mathbf{k}\sigma}$ calculated exactly (not shown) and by RMFT are identical due to Eq. (6).

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 $|N_e\pm1\rangle$, we calculate their excitation energies for each momentum and also the corresponding energy gap by fitting the excitation energy $E_{\mathbf{k}}$. To reduce the effect of finite size, we define the sum of $Z^{\pm}_{\mathbf{k}\sigma}/N$, over momentum $\mathbf{k}$ 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 an energy interval 0.2 for various dopings.[25] To make sure our treatment is correct, we

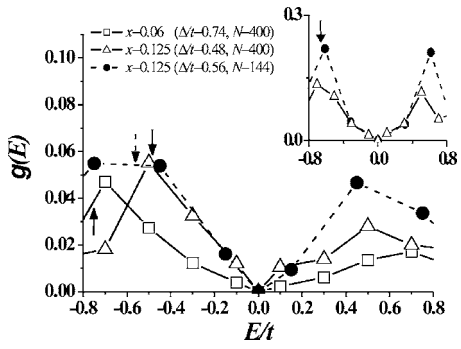

FIG. 3. $g(E)$ for d-RVB state versus excitation energy E for 12×12 (solid circle) and 20×20 lattices (empty square and triangle, for different dopings). The associated excitation gap positions are marked by arrows (see text). **Inset**: Same plots for d-BCS state with gap value 0.6 and $x=0.125$. The data shown here are for different sizes, denoted by the same symbols as in the main figure, with parameters $\mu/t=-0.269$ (12×12) and $\mu/t=-0.272$ (20×20), respectively. All data are obtained for $(t',t'')/t=(-0.3,0.2)$.

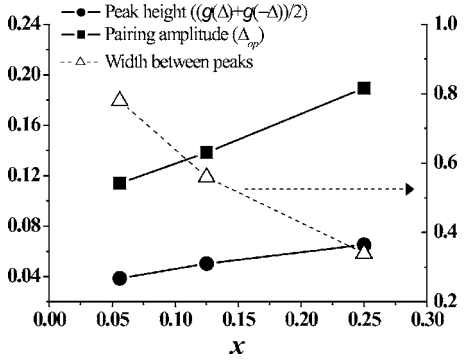

FIG. 4. The doping dependence of the peak height for $g(E)$, pairing amplitude and width between peaks in 20×20 lattice for d-RVB case. Data are extracted from that shown in Fig. 3 and those obtained in the same way but not shown there. The values for the width between peaks are referred to the vertical axis on the right-hand side (indicated by the arrow).

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 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 Δ (in units of t) increases from 1.96 to 2.73 (Ref. 23). 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 tell us the 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.

Figure 3 also reveals the correlation between the heights of the spectral weight peak and the gap size (or the width between peaks) as the doping level is varied.[23] Within the doping level shown in Fig. 4, the peak height scales with the pairing amplitude but apparently anticorrelates with the gap size. This is in clear contrast to the BCS case in which the peak height, proportional to the SC coherence, scales with the width between the peaks or gap size as more holes are doped into the system. Our result agrees qualitatively with what has been extracted from STS experiments.[5]

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 the pairing amplitude and SW products. Performing a

particle-hole transformation, we also obtain 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 the SW peaks anticorrelates with the peak heights.

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