Low-Energy Spectra in t-J-Type Models at Low Doping Levels

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Based on a variational approach, we propose that there are two kinds of low-energy states in the t-J-type models at low doping. In a quasiparticle state an unpaired spin bound to a hole with a well-defined momentum can be excited with spin waves. The resulting state shows a suppression of antiferromagnetic order around the hole with the profile of a *spin bag*. These spin-bag states with spin and charge or hole separated form a continuum of low-energy excitations. Very different properties predicted by these two kinds of states explain a number of anomalous results observed in the exact diagonalization studies on small clusters up to 32 sites.

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Soon after the discovery of the high T_c superconducting cuprates, the t-J model was proposed [1] as the prototype to examine the phenomena. Since then it has been shown [2–5] that extra hoppings beyond nearest neighbors (nn) are also important to the low-energy features of the cuprates. Enormous theoretical effort has been devoted to predict the low-energy spectra of these t-J-type models. But the strong correlation associated with these models has made perturbative approaches ineffective. With the many different mean-field theories presented so far, there is little consensus to the "correct" description of low-energy spectra of these models. To sort out the proper theory it is important to first have a detailed comparison of the predictions with the results of exact calculations.

Recently, significant progress has been made at very low doping. Several different numerical techniques, such as exact diagonalization (ED) studies [6–8], self-consistent Born approximation [9], and the Green function Monte Carlo method [10], all have obtained similar results for the energy-momentum dispersion relation of a single hole doped into t-J-type models. The results agree fairly well with experiments [5]. In addition, a mean-field or variational wave function (VWF) [11] constructed from the half-filled Mott insulating state with antiferromagnetic long-range order (AF LRO) has also obtained a similar success. In Ref. [3] this single-hole VWF is generalized to treat systems with multiple holes or electrons. The new set of VWF's easily explained angle-resolved photoemission spectroscopy (ARPES) results [4] for Fermi pockets around $(\pi/2, \pi/2)$ and $(\pi, 0)$ for hole-doped and electron-doped systems, respectively. It [3] also reproduced unusual patterns in momentum distribution functions (MDF's) of the ground state calculated by the ED method [12,13] for one and two holes in 32 sites. For these VWF's, doped holes or electrons behave like quasiparticles (QP's). In this Letter we show that in addition to these QP states, there is a continuum of excitations described by *spin-charge separated* states in the spectra of t-J-type models. The presence of the two kinds of states is carefully examined by explaining several anomalous results reported by ED studies for clusters up to 32 sites.

As shown by Lee *et al.* [3], the ground state in the presence of a few doped holes or electrons could be described by a VWF constructed from the half-filled Mott insulating state. At half filling, the ground state is described fairly accurately by including three mean-field parameters [11,14]: the staggered magnetization $m_s = \langle S_A^z \rangle = -\langle S_B^z \rangle$, where the lattice is divided into A and B sublattices; the uniform bond order parameters $\chi = \langle \sum_\sigma c_{i\sigma}^\dagger c_{j\sigma} \rangle$; and d-wave resonating valence bond (d-RVB) order $\Delta = \langle c_{j\downarrow} c_{i\uparrow} - c_{j\uparrow} c_{i\downarrow} \rangle$ if i and j are nn sites in the x direction and $-\Delta$ for the y direction. Without d-RVB order, the mean-field Hamiltonian has lower and upper spin-density-wave (SDW) bands with operators $a_{\mathbf{k}\sigma} = \alpha_{\mathbf{k}} c_{\mathbf{k}\sigma} + \sigma \beta_{\mathbf{k}} c_{\mathbf{k}+\mathbf{Q}\sigma}$, and $b_{\mathbf{k}\sigma} = -\sigma \beta_{\mathbf{k}} c_{\mathbf{k}\sigma} + \alpha_{\mathbf{k}} c_{\mathbf{k}+\mathbf{Q}\sigma}$, respectively. Here $\mathbf{Q} = (\pi, \pi)$, $\alpha_{\mathbf{k}}^2 = \frac{1}{2}[1 - (\epsilon_{\mathbf{k}}/\xi_{\mathbf{k}})]$, and $\beta_{\mathbf{k}}^2 = \frac{1}{2}[1 + (\epsilon_{\mathbf{k}}/\xi_{\mathbf{k}})]$. Energy dispersions for the two SDW bands are $\pm\xi_{\mathbf{k}} = \pm[\epsilon_{\mathbf{k}}^2 + (Jm_s)^2]^{1/2}$ with $\epsilon_{\mathbf{k}} = -\frac{3}{4} J\chi(\cos k_x + \cos k_y)$. Inclusion of d-RVB pairing for electrons on total N_s sites, the VWF for the ground state has the form $|\Psi_0\rangle = P_e[\sum_{\mathbf{k}}(A_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger + B_{\mathbf{k}} b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger)]^{N_s/2}|0\rangle$, where $A_{\mathbf{k}} = (E_{\mathbf{k}} + \xi_{\mathbf{k}})/\Delta_{\mathbf{k}}$ and $B_{\mathbf{k}} = -(E_{\mathbf{k}} - \xi_{\mathbf{k}})/\Delta_{\mathbf{k}}$ with $E_{\mathbf{k}} = (\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2)^{1/2}$ and the constraint of one electron per site enforced by P_e. Here $\Delta_{\mathbf{k}} = \frac{3}{4} J\Delta(\cos k_x - \cos k_y)$. The sum in $|\Psi_0\rangle$ is taken over the sublattice Brillouin zone (SBZ).

In the presence of doped holes or electrons, we consider the t-J-type model including longer-ranged hoppings, with amplitues t' for the second nn and t'' for the third nn. By applying a particle-hole transformation [3,6] we can treat hole- and electron-doped cases in the same manner. However, here we concentrate only on the hole-doped cases with $J/t = 0.3 = -t'/t$ and $t''/t = 0.2$.

When a hole is doped or an electron is removed from $|\Psi_0\rangle$, a pair must be broken with an unpaired spin left. Thus it is quite natural to have the following VWF [3,11] for a single doped hole, e.g., with a lone up spin

$$|\Psi_1(\mathbf{q}_s)\rangle = P_d c^{\dagger}_{\mathbf{q}_s\uparrow}\Big[\sum_{[\mathbf{k}\neq\mathbf{q}_h]}(A_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\uparrow}a^{\dagger}_{-\mathbf{k}\downarrow} + B_{\mathbf{k}} b^{\dagger}_{\mathbf{k}\uparrow}b^{\dagger}_{-\mathbf{k}\downarrow})\Big]^{(N_s/2)-1}|0\rangle,$$

where the hole momentum $\mathbf{q}_h$ is excluded from the sum if $\mathbf{q}_h$ is within the SBZ; otherwise, $\mathbf{q}_h - \mathbf{Q}$ is excluded. P_d here enforces the constraint of no doubly occupied sites. When we choose the unpaired-spin momentum $\mathbf{q}_s$ to be the same as either the hole momentum $\mathbf{q}_h$ or $\mathbf{q}_h + \mathbf{Q}$, this VWF is equivalent to the Lee-Shih [11] one. Variational energies calculated vary with $\mathbf{q}_h$ [3,11]. The energy dispersions for t-J and t-t'-t''-J models are plotted as filled circles in Figs. 1(a) and 1(b), respectively. For both models, the ground state with one hole has momentum $(\pi/2, \pi/2) \equiv \mathbf{Q}/2$. As shown in Ref. [3], these dispersion relations are still followed when the hole number is increased. The holes in these wave functions behave just like QP's; hence we denote $|\Psi_1(\mathbf{q}_h = \mathbf{q}_s)\rangle \equiv |\Psi_1^{\mathrm{QP}}\rangle$.

There are only two variational parameters: Δ/χ and m_s/χ in our VWF's. The extended hoppings t' and t'' are not used as variational parameters in both $|\Psi_1^{\mathrm{QP}}\rangle$ and $|\Psi_1\rangle$.

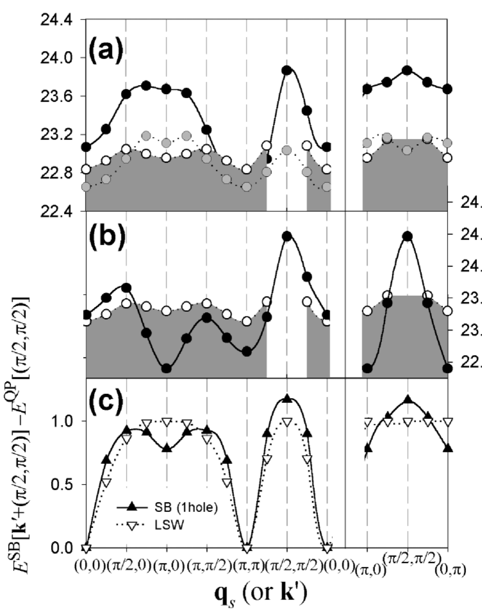

FIG. 1. Variational energies calculated for the (a) t-J and (b) t-t'-t''-J model Hamiltonians for one hole on an 8×8 lattice by applying our VWF's. Filled circles, connected by solid lines, are variational results using the $|\Psi_1^{\mathrm{QP}}(\mathbf{q}_s)\rangle$ discussed in the text; empty (gray) circles by $|\Psi_1^{\mathrm{SB}}[\mathbf{q}_s, \mathbf{q}_h = \mathbf{Q}/2^M((3\pi/4, 0))]\rangle$. Shaded regions indicate a possible continuum for an infinite system. A minus sign has been multiplied to all the data shown here. (c) Difference of variational energies between the QP ground state at $\mathbf{Q}/2$ and the SB states at $\mathbf{q}_s = \mathbf{Q}/2 + \mathbf{k}'$ in (b) as a function of $\mathbf{k}'$. The dotted line is the prediction of energy dispersion of linear spin-wave theory [16]. Results here are obtained with parameters $(\Delta/\chi, m_s/\chi) = (0.25, 0.125)$.

Clearly, the choice of unpaired spin to have the same momentum as the hole, i.e., $\mathbf{q}_s = \mathbf{q}_h$, is a special case for $|\Psi_1\rangle$. If we choose $\mathbf{q}_s \neq \mathbf{q}_h$, then not only the electron pair at $\mathbf{q}_h$ and $-\mathbf{q}_h$ is excluded in the sum in $|\Psi_1\rangle$, the pair at $\mathbf{q}_s$ and $-\mathbf{q}_s$ is also affected. Hence we expect it to be higher in energy. To make a distinction from the aforementioned QP states $|\Psi_1^{\mathrm{QP}}\rangle$, these states are denoted as the *spin-bag* (SB) states, i.e., $|\Psi_1(\mathbf{q}_s \neq \mathbf{q}_h)\rangle \equiv |\Psi_1^{\mathrm{SB}}\rangle$. The variational energies as a function of $\mathbf{q}_s$ for $|\Psi_1^{\mathrm{SB}}\rangle$ with $\mathbf{q}_h = \mathbf{Q}/2$ are plotted as empty circles in Figs. 1(a) and 1(b) for the t-J and t-t'-t''-J models, respectively. Many SB states could be constructed with the same $\mathbf{q}_s$ but different $\mathbf{q}_h$. While it is possible to have the SB states of even lower energy with $\mathbf{q}_h = (3\pi/4, 0)$ in the t-J model [gray circles in Fig. 1(a)], they are of higher energies than that of SB states with $\mathbf{q}_h = (\pi/2, \pm\pi/2)$ in the t-t'-t''-J case. There are many such states, actually an infinite number of them for an infinite system, forming a continuum, as schematically illustrated by the shaded regions in Figs. 1(a) and 1(b).

There is an intuitive way to understand the difference between SB and QP states. The spin excitations of the QP states can be easily constructed by applying the spin operators, $S^{\dagger(-)}(\mathbf{k}') = \sum_{\mathbf{q}'} c^{\dagger}_{\mathbf{q}'+\mathbf{k}'\uparrow(\downarrow)} c_{\mathbf{q}'\downarrow(\uparrow)}$, to $|\Psi_1^{\mathrm{QP}}\rangle$. In the linear spin-wave theory $\mathbf{k}'$ is the momentum of the spin wave. The particular term included in the sum of $\mathbf{q}'$ with $\mathbf{q}'$ equal to the momentum of the unpaired spin $\mathbf{q}_s = \mathbf{q}_h$ changes the QP state $|\Psi_1^{\mathrm{QP}}\rangle$ to the SB ones $|\Psi_1^{\mathrm{SB}}(\mathbf{q}_s = \mathbf{q}_h + \mathbf{k}')\rangle$. Thus the SB states are actually just spin-wave excitations of the QP state with the same hole momentum. In Fig. 1(c) the difference of variational energies between the SB states and the QP state with $\mathbf{q}_h = \mathbf{Q}/2$ for the t-t'-t''-J model is plotted as a function of the difference of momentum $\mathbf{k}' = \mathbf{q}_s - \mathbf{q}_h$. The dotted line is the prediction of energy-momentum dispersion relation of linear spin-wave theory [15]. The slight differences between the two results at $\mathbf{k}' = \mathbf{Q}/2$ and $\mathbf{k}' = (\pi, 0)$ are due to the hole-renormalization effect [16]. SB states represent spin excitations of the QP states. The gray [empty] circles in Fig. 1(a) [1(b)] are the lowest spin excitation energies of the ground state [17].

The two VWF's also give very different spin and hole correlations. In Fig. 2 we show the correlation functions $SH_A(\mathbf{r}) = \sum_{i\in A}(-1)^{i+\mathbf{r}}\langle\Psi_1|n_i^h S^z_{i+\mathbf{r}}|\Psi_1\rangle / \sum_{i\in A}\langle\Psi_1|n_i^h|\Psi_1\rangle$, for a QP state (filled triangles) with $\mathbf{q}_s = \mathbf{q}_h = (0,0)$ and a SB state (empty triangles) with $\mathbf{q}_s = (0,0)$ and $\mathbf{q}_h = \mathbf{Q}/2$ [18]. $SH_{A(B)}$ is for the hole at the $A(B)$ sublattice and n_i^h the hole-number operator at site i. In our convention, the up spin prefers to be on sublattice A. If the hole and unpaired spin are uncorrelated, $SH_{A(B)}$ equals to the value of uniform staggered magnetization. Even though both states have an unpaired down spin and a single hole, the spin configurations around the hole are clearly different. The spin magnetization right next to the hole in the QP state $|\Psi_1^{\mathrm{QP}}\rangle$ has values larger than the uniform background, 0.368. Thus

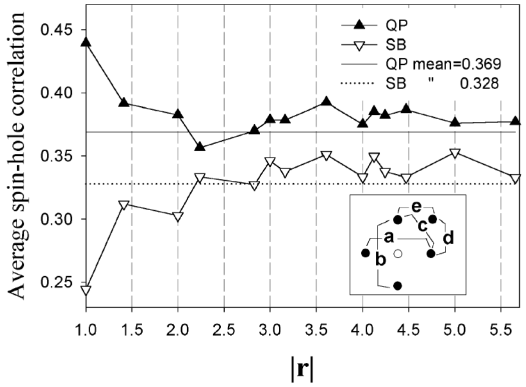

FIG. 2. Spin-hole correlation functions, SH_A (defined in the text), calculated using the QP state (filled triangles) with $\mathbf{q}_s = \mathbf{q}_h = (0,0)$ and the SB state (empty triangles) with $\mathbf{q}_s = (0,0)$ and $\mathbf{q}_h = \mathbf{Q}/2$ [19] with the same parameters used in Fig. 1. Inset: pairs of sites, denoted by letters **a** to **e**, where spin-spin correlations listed in Table I are computed.

the unpaired spin is bound to the hole. On the other hand, for the SB state the magnetization is suppressed around the hole; this is similar to the idea of a SB first proposed in Ref. [19]. The unpaired spin bound to the hole in the QP state is here excited by the spin-wave excitation and becomes unbound in the SB state. This may be viewed as a spin-charge separated state.

The spin-charge separation observed in the SB states has many interesting consequences. In ED studies, it has been found[20] that the lowest energy state at $(\pi, 0)$ for the t-t'-t''-J model is very different from that of the t-J model. The spin-spin correlation across the hole changes from ferromagnetic (FM) to AF when t' is turned on. This result can now be understood as follows: the lowest energy state at $(\pi, 0)$ for the t-J model is the QP state $|\Psi_1^{\mathrm{QP}}[\mathbf{q}_s = \mathbf{q}_h = (\pi, 0)]\rangle$ as shown in Fig. 1(a), but it changes to a SB state $|\Psi_1^{\mathrm{SB}}(\mathbf{q}_s = (\pi, 0), \mathbf{q}_h = \mathbf{Q}/2)\rangle$ for the t-t'-t''-J model as shown in Fig. 1(b). In Table I we list correlations obtained between pairs of spins around the doped hole for QP and SB states. The correlation is defined as $C_{\delta,\delta'}(\mathbf{q}_s) \equiv \sum_i \langle \Psi_1^{\mathrm{QP,SB}}(\mathbf{q}_s)| n_i^h \mathbf{S}_{i+\delta} \cdot \mathbf{S}_{i+\delta'} |\Psi_1^{\mathrm{QP,SB}}(\mathbf{q}_s)\rangle$ with δ and δ' denoting two sites around the hole[20]. While the lower-energy QP states at $\mathbf{q}_s = \mathbf{q}_h = (\pi, 0)$ and $(0, 0)$ behave as expected for a system with AF LRO, i.e., FM for spins at the same sublattice (pairs **a** and **b**) and AF otherwise, the result for a SB state with $\mathbf{q}_s = (\pi, 0)$ and $\mathbf{q}_h = \mathbf{Q}/2$ shows AF correlation at the same sublattice This is exactly the behavior observed in ED results [20]. Our result in Fig. 1 shows that at $(0, 0)$ the lowest energy state remains to be the QP state even when t' and t'' are included. The spin correlations are thus not changed; this is also consistent with what is found by Tohyama *et al.* [20].

TABLE I. $C_{\delta,\delta'}(\mathbf{q}_s)$ calculated for an 8×8 lattice using different VWF's with momenta indicated. The first and third rows are for QP states while others are for SB ones. **a** to **e** are different pairs of sites defined in the inset of Fig. 2. Positive (negative) values mean FM (AF) correlations.

$\mathbf{q}_s$	$\mathbf{q}_h$	a	b	c	d	e
$(0,0)$	$(0,0)$	0.188	0.188	0.202	-0.273	-0.264
$(0,0)$	$\mathbf{Q}/2$	-0.0288	-0.0254	-0.0302	-0.203	-0.195
$(\pi,0)$	$(\pi,0)$	0.123	0.15	0.071	-0.353	-0.279
$(\pi,0)$	$\mathbf{Q}/2$	-0.0313	-0.0085	-0.002	-0.1921	-0.212

Another important difference between QP and SB states is in their MDF $\langle n_\sigma(\mathbf{k})\rangle$. Since $\mathbf{q}_h$ is excluded from the VWF $|\Psi_1\rangle$, we naturally expect $\langle n_\uparrow(\mathbf{k})\rangle$ to have a smaller value or a dip at $\mathbf{k} = \mathbf{q}_h$ and $\mathbf{k} = \mathbf{q}_h + \mathbf{Q}$ than its neighbors, similarly for $\langle n_\downarrow(\mathbf{k})\rangle$ at $\mathbf{k} = -\mathbf{q}_h$ and $\mathbf{k} = -\mathbf{q}_h + \mathbf{Q}$. However, in a QP state with an up spin at momentum $\mathbf{q}_s = \mathbf{q}_h$, then $\langle n_\uparrow(\mathbf{k} = \mathbf{q}_h)\rangle$ is increased and there is no more a dip. As an example, the MDF obtained by the QP state with $\mathbf{q}_h = \mathbf{q}_s = (\pi, 0)$ is listed in Fig. 3(a). Because of the symmetry, only results for one quadrant of the BZ are shown. At each $\mathbf{k}$ the upper (lower) number is for up (down) spin. Now for a SB state with a lone up spin at $\mathbf{q}_s (\neq \mathbf{q}_h)$, the original spin at $\mathbf{q}_h$ in the QP state is excited and placed at $\mathbf{q}_s$; then $\langle n_\uparrow(\mathbf{k} = \mathbf{q}_h)\rangle$ still has a dip. Figure 3(b) shows the MDF obtained for the SB state with $\mathbf{q}_s = (\pi, 0)$ and $\mathbf{q}_h = \mathbf{Q}/2$ [18]. Results are here for 32 sites and $(\Delta/\chi, m_s/\chi) = (0.1, 0.05)$.

This behavior of the MDF's is indeed found in the exact results for the lowest energy state at $(\pi, 0)$ of the t-J and t-t'-t''-J models as shown in Figs. 3(c) and 3(d), respectively. The nice qualitative agreement achieved between Figs. 3(a) and 3(c) as well as between 3(b) and 3(d) reaffirms our results shown in Figs. 1(a) and 1(b): the

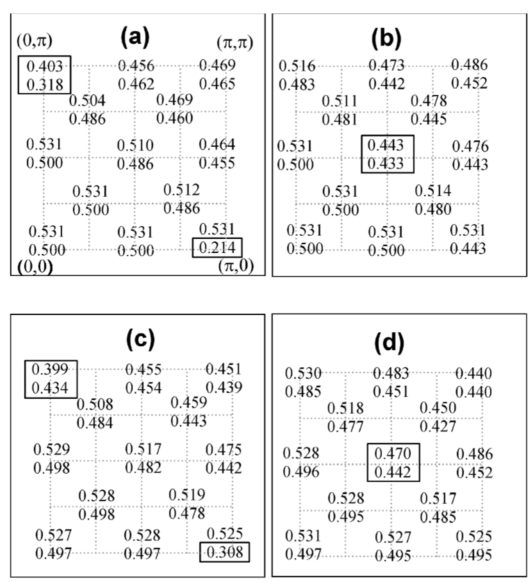

FIG. 3. Momentum distribution functions in one quadrant of the BZ for 32 sites obtained by (a) $|\Psi_1^{\mathrm{QP}}(\mathbf{q} = (\pi, 0))\rangle$, (b) $|\Psi_1^{\mathrm{SB}}(\mathbf{q}_s = (\pi, 0), \mathbf{q}_h = \mathbf{Q}/2)\rangle$, (c) ED results for the $(\pi, 0)$ state of the t-J model and (d) the t-t'-t''-J model. The upper number is the result for up spin and the lower for down spin.

lowest energy state at $(\pi, 0)$ for a single hole is a QP state for the t-J model and a SB state for the t-t'-t''-J model.

Another consequence of this switch from a QP state to a SB one is the drastic change of the spectral weight, $Z_{\mathbf{k}} = |\langle\Psi_1(\mathbf{k})|c_{\mathbf{k}\sigma}|\Psi_0\rangle|^2/\langle\Psi_0|c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|\Psi_0\rangle$. We obtained $Z_{\mathbf{k}} = 0.475$ and 0.0 by using $|\Psi_1^{\mathrm{QP}}(\mathbf{q} = (\pi, 0))\rangle$ and $|\Psi_1^{\mathrm{SB}}(\mathbf{q}_s = (\pi, 0), \mathbf{q}_h = \mathbf{Q}/2)\rangle$, respectively. This is consistent with exact results for the t-J model ($Z_{\mathbf{k}} = 0.34$)[7] and the t-t'-t''-J model ($Z_{\mathbf{k}} = 0$) [21]. In addition, spectral weights of the lowest energy states of both models at (π, π) and $(3\pi/4, 3\pi/4)$ are either exactly zero or very small. This is consistent with our identification that states at both momenta are SB ones. Since $c_{\mathbf{k}\sigma}|\Psi_0\rangle$, unlike the SB state, has momenta of the hole and unpaired spin related, it has a negligible overlap with the SB state. By contrast, states at $(\pi/2, \pi/2)$ and $(\pi/4, \pi/4)$ remain to be QP states in both t-J and t-t'-t''-J models; hence large spectral weights are expected. It is noted that our QP (SB) states predict larger (smaller) spectral weights in comparison with that of the exact 32 sites. This discrepency is partly due to the fact that we have AF LRO in our VWF's while total spin is a good quantum number in the exact results. Another reason is that due to the projection operator P_d our QP states and SB states with the same quantum numbers (total momentum and total S_z) are actually not orthogonal to each other although they have very small overlap. But there are many SB states in the continuum that could couple with a particular QP state. Hence, when the QP state has energies very close to the continuum, the spectral weight of the QP state is diluted by the coupling with SB states. This effect makes the quantitative prediction of spectral weight difficult. We leave this issue for the future work.

In summary, based on a mean-field theory with AF and d-RVB order parameters we have proposed that at low doping there are two kinds of low-energy states for t-J-type models. The single-hole QP states have a well-defined energy dispersion. By exciting the QP states with spin waves we obtain a continuum of SB states. The unpaired spin is separated from the hole in the SB states. A number of physical properties predicted by these two kinds of states are in good agreement with the exact results obtained by ED studies. Although our emphasis in this Letter is to show the solid theoretical support of these two kinds of states, there are also experimental evidences. In Ref. [3], QP states were shown to explain well the single-hole dispersion observed by ARPES. However, the overall variation pattern of spectral weights observed in the ARPES experiment on $Ca_2CuO_2Cl_2$ [4] is naturally understood with the presence of SB states: notable lowest energy peaks are observed only in small regions of k space, e.g., near $(\pi/2, \pi/2)$ and $(\pi/2, 0)$ where QP states have lower energy than the SB states [Fig. 1(b)]. More comparison with experiments is in progress.

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[18] Notice that results for SB states are average over the two degenerate ones with $\mathbf{q}_h = (\pi/2, \pi/2)$ and $\mathbf{q}_h = (\pi/2, -\pi/2)$.

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[21] Note that the $(\pi, 0)$ state reported in Ref. [7] is *not* the lowest energy state with the same momentum. The lowest one which was omitted has zero overlap with $c_{\mathbf{k}\sigma}|\Psi_0\rangle$ and, consequently, $Z_{\mathbf{k}} = 0$.