Theory of a single Oxygen hole propagating in Sr$_2$CuO$_2$Cl$_2$: the spin of the quasiparticles in CuO$_2$ planes

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Abstract

Recent photoemission experiments have measured $E$ vs. $\vec{k}$ for a single hole propagating in antiferromagnetically aligned $\text{Sr}_2\text{CuO}_2\text{Cl}_2$. Comparisons with (i) the $t - t' - J$ model, for which the carrier is a spinless vacancy, and (ii) a strong-coupling version of the three-band Emery model, for which the carrier is a $S = \frac{1}{2}$ hole moving on the Oxygen sublattice, have demonstrated that if one wishes to describe the quasiparticle throughout the entire first Brillouin zone the three-band model is superior. Here we present a new variational wave function for a single Oxygen hole in the three-band model: it utilizes a classical representation of the antiferromagnetically ordered Cu-spin background but explicitly includes the quantum fluctuations of the lowest energy doublet of the Cu-O-Cu bond containing the Oxygen hole. We find that this wave function leads to a quasiparticle dispersion for physical exchange and hopping parameters that is in excellent agreement with the measured ARPES data. We also obtain the average spin of the Oxygen hole, and thus deduce that this spin is only quenched to zero at certain wave vectors, helping to explain the inadequacy of the $t - t' - J$ model to match the experimentally observed dispersion relation everywhere in the first Brillouin zone.

Keywords: Strongly correlated electronic systems; high $T_c$ CuO$_2$ planes; 3-band Hubbard model
1. INTRODUCTION

The high $T_c$ transition metal oxides have been intensely studied, with the focus of most researchers directed towards the physics of the CuO$_2$ planes. Undoped, these planes are composed of $S = \frac{1}{2}$ spins at each Cu site, and it has been shown that a simple Heisenberg Hamiltonian with a near-neighbour exchange of the order of 1500 K provides an excellent representation of the antiferromagnetic (AFM) interactions between the spins over a wide temperature range [1].

Having confidence in a good model of the undoped state, a theory must be developed dealing with the motion of carriers in a Cu–spin background. Upon doping the planes mobile holes are produced, and these holes are known to predominantly occupy the Oxygen sites in the CuO$_2$ planes. However, Anderson first proposed that one–band models are sufficient to represent the important low–energy physics of such carrier motion [2]. This proposition was formalized in work by Zhang and Rice [3], and later by Shastry [4]: starting from a three–band Hubbard model they delineated how it is possible to map the Oxygen hole motion onto a one–band $t – t' – J$ model (in fact, in Shastry’s formulation, hopping processes connecting sites that are further than next–nearest–neighbour are allowed). It is to be emphasized that at the end of this renormalization, the spin degree of freedom of the Oxygen carrier described by the three–band Hubbard model is quenched, and the carrier described by the $t – t' – J$ model is a spinless vacancy. While this renormalization has been the subject of some debate, no definitive experimental data have allowed for one to say that the one–band model is indeed a viable representation of carrier motion. Instead, one–band model researchers are forced to adopt something similar to the following posture: the physics of the $t – t' – J$ model is sufficiently difficult to warrant the attention of a high $T_c$ theorist, and hopefully the physics of the superconducting instability and the anomalous normal state will be contained in this model.

Fortunately, recent experimental work does allow for careful qualitative and quantitative scrutiny of this assumption. To be specific, angle–resolved photoemission spectroscopy
(ARPES) of insulating Sr$_2$CuO$_2$Cl$_2$ was recently completed [5]. This experiment presents theorists with, for the first time, data for the spectral function of a single hole propagating in a CuO$_2$ plane. In fact, Sr$_2$CuO$_2$Cl$_2$ is an ideal model system to obtain such data since complications associated with the orthorhombicity of many high $T_c$ materials can be avoided — Sr$_2$CuO$_2$Cl$_2$ does not undergo such a structural phase transition until about 10 K and reliable ARPES data were collected at 350 K.

Subsequent to this work, a comparison of the $t - t' - J$ model’s $E$ vs. $\vec{k}$ results to the ARPES data of Ref. [5] displayed that the one–band model did not reproduce the bandstructure everywhere in the AFM Brillouin zone [6]. Instead, in this same paper [6], we summarized our results showing that the three–band model in the strong–coupling limit did a superb job of reproducing the $E$ vs. $\vec{k}$ ARPES data for all wave vectors. Here we elaborate on that work and also display a new, more detailed comparison to experiment.

In this paper we focus on a model of Oxygen holes moving in a CuO$_2$ plane. A new variational wave function for this problem is introduced and applied to the Sr$_2$CuO$_2$Cl$_2$ ARPES data. This variational wave function is similar in spirit to the successful semi–classical variational wave functions introduced by Shraiman and Siggia for the one–band model [7] and later generalized to the three–band model [8]. However, unlike the variational wave function of Ref. [8], here we include the lowest–order quantum fluctuations of the occupied Cu–O–Cu bond, thus allowing for the so–called trion quasiparticle [9] to be accounted for. These quantum fluctuations permit, in principle, for the spin of the Oxygen hole to be quenched to zero, an essential ingredient in the Zhang–Rice renormalization [3] of the three–band Hubbard model to the one–band $t - t' - J$ model.

We show that our new variational wave function for a single Oxygen hole provides an excellent representation of the $E$ vs. $\vec{k}$ relation measured in Ref. [5] for physically reasonable exchange and hopping parameters. We then analyze these wave functions and show that unlike the result of the renormalization of the three–band to the one–band model, the spin of the carrier is not quenched to zero everywhere in the Brillouin zone. This thus provides us with an understanding of the inability of the $t - t' - J$ model to reproduce the $E$ vs. $\vec{k}$
Further analysis has allowed us to reduce this quasiparticle to that of a doublet (the ground state of three $S=\frac{1}{2}$ spins antiferromagnetically coupled, as in the occupied Cu–O–Cu bond) moving in a distorted Néel background of Cu spins, viz., the trion quasiparticle of Ref. [9].

Our paper is organized as follows. In §2 we describe the components of the three–band model in the strong–coupling limit. In §3 we present our new variational wave function, a description particular to the three–band model and one that contains some quantum fluctuations of the propagating Oxygen hole. This section also contains a comparison of our results to the ARPES data of Ref. [5]. Section 4 presents an analysis of the wave function that results from the fit to the ARPES data, including the nature and spin of the quasiparticle. Finally, §5 summarizes our main findings and describes future work on this problem.

## 2. COMPONENTS OF THE THREE–BAND HAMILTONIAN

The application of the extended three–band Hubbard model to a description of the CuO$_2$ planes of the high $T_c$ oxides was first discussed by Emery [10] and Varma et al. [11]. The parameters that are believed to enter this model have been evaluated elsewhere [12,13]. Here we simply note that if one takes a 3d$^{10}$2p$^6$ configuration as the vacuum state, then in the strong–coupling limit one can derive the following Hamiltonian as representative of the motion of Oxygen holes in a Cu–spin background [12,13]:

$$
\hat{H} = J_{Cu-Cu} \sum_{\langle i,i' \rangle} \left( \vec{S}_i \cdot \vec{S}_{i'} - 1/4 \right) + J_{Cu-O} \sum_{\langle i,l \rangle} \left( \vec{S}_i \cdot \vec{S}_l - \frac{1}{4} n_l \right) + (t_a + t_b) \sum_{\langle l,l' \rangle, \sigma, \sigma'} \left( \vec{S}_i \cdot \left( b^\dagger_{l',\sigma'} \vec{\tau}_{\sigma',\sigma} b_{l,\sigma} \right) + h.c. \right) + \frac{1}{2} (t_b - t_a) \sum_{\langle l,l' \rangle, \sigma} \left( b^\dagger_{l,\sigma} b_{l',\sigma} + h.c. \right) - |t_{pp}| \sum_{\langle l,l' \rangle, \sigma} (b^\dagger_{l,\sigma} b_{l',\sigma} + h.c.).
$$

(1)

In this equation $i$ refers to Copper sites and $l$ refers to Oxygen sites; the $\vec{S}_i$ are the Cu spin operators, whereas the spin operator for an Oxygen hole is $\vec{S}_l = \frac{1}{2} b^\dagger_{l,\sigma} \vec{\tau}_{\sigma,\sigma'} b_{l,\sigma'}$, where $\vec{\tau}_{\sigma,\sigma'}$ are the Pauli matrices, and $b_{l,\sigma}$ is the destruction operator for an Oxygen hole that...
precludes double occupancy. The primed summation indicates that the superexchange is not calculated for the bond containing the Oxygen hole. The $t_a$ hopping process corresponds to the Oxygen hole passing through a Cu site without affecting the Cu hole, whereas the $t_b$ hopping exchanges the carrier with the hole of a Cu site — a more detailed description of the hopping processes and notation for this Hamiltonian are provided in Ref. [8]. Implicit in Eq. (1) is the reduction of all Oxygen $p$ and Cu $d$ orbitals to one’s having an effective $s$–wave character — e.g., see Ref. [9].

The Cu–Cu superexchange parameter has been measured to be 0.125 eV [1], and here we fix $J_{Cu-Cu} = 0.125$ eV. Further, it has been argued [8,9] that $J_{Cu-O}/J_{Cu-Cu} \sim 4 \rightarrow 6$, and thus we fix $J_{Cu-O} = 0.63$ eV [14]. To estimate the hopping energies, perturbation theory [8,9] and electronic structure work [12,13] may be used. (In the perturbation theory we have used a reduced $pd$ energy overlap integral $t_{pd} = 1.25$ eV to account, in a first–order fashion, for the larger lattice constant of Sr$_2$CuO$_2$Cl$_2$ — this value, when employed with perturbation theory, accurately predicts the Cu–Cu superexchange.) We find

$$t_a \sim 0.32 \text{ eV}, \quad t_b \sim 0.36 \text{ eV}, \quad \text{and} \quad t_{pp} \sim -0.65 \text{ eV}.$$ (2)

These numbers are similar to other published sets of estimates.

We have chosen to fix both the experimentally determined $J_{Cu-Cu}$, as well as our value of $J_{Cu-O} = 0.63$ eV (varying $J_{Cu-O}$ by ±25 per cent does not affect our results). However, the other parameters we allow to become fitting parameters, and we choose them by fitting to the $E \ vs. \vec{k}$ ARPES data. Of course, if our fitted parameters are too far from those expressed in Eq. (2) then it is not at all clear that our fits are in any way physically reasonable. Fortunately, we find reasonably close agreement with these numbers.

### 3. NEW VARIATIONAL WAVE FUNCTION

One successful approach [7] to the problem of a vacancy moving in an AFM background described by the $t – J$ model was proposed by Shraiman and Siggia. In their formalism
the undoped state corresponds to a classical AFM, a state which has as its wave function a simple product of spinors. Then they suggested that one way to determine the symmetry and spin texture of the singly–doped ground state involved taking a semiclassical variational wave function based on a product state of spinors representing (again) a classical Cu–spin background that included a single vacancy. Bloch states can be formed from this product state, and then the direction of each individual spin (relative to the position of the vacancy) was determined by the variational principle, namely (figuratively speaking) by allowing for the delocalization of the hole without costing too much magnetic exchange energy. It is to be stressed that even though the exchange interactions are treated using classical spins, the vacancy is placed in a Bloch state and as it moves throughout the lattice the quantum–mechanical overlaps of the spins are fully accounted for. A detailed account and summary of the results and predictions of the field theory that results from this work can be found in Ref. [15].

The extrapolation of this idea to the strong–coupling three–band Hamiltonian of Eq. (1) was carried out by Frenkel, one of the present authors, and Shraiman and Siggia [8]. However, when we applied the type of variational wave function developed in Ref. [8] to the $E$ vs.$\vec{k}$ ARPES data of Ref. [5], we found that our fits led to ridiculous hopping energies [6]. Thus, we have produced a new variational wave function which we feel better approximates the physics of the carrier motion of an Oxygen hole in a CuO$_2$ plane.

To introduce our wave function it is instructive to first state the wave function that was developed and studied in Ref. [8]. The Shraiman–Siggia–type wave functions incorporate the broken symmetry of the AFM lattice; thus, referring to Fig. 1, for a model that includes both the Cu and Oxygen sites there are two Cu basis sites (the spin up and spin down sublattices of the AFM) and four Oxygen basis sites per primitive unit cell. Labeling the Cu sites by their position with respect to the unit cell in which the Oxygen hole resides, viz., the unit cell denoted by $\vec{r}$, one may write the wave function in the following form:

$$|\Psi_{\vec{k}}\rangle = \sum_{\vec{r}} e^{i\vec{k} \cdot \vec{r}} \sum_{\mu=1}^{4} \gamma_{\mu} \psi_{\mu}^{O}(\vec{r}) \prod_{i} \psi_{\mu}(\vec{r}_{i} - \vec{r}) \psi_{\mu}(\vec{r}_{i} + \hat{x} - \vec{r})$$ \quad (3)
In this equation, \( i \) labels the primitive unit cells and \( \vec{r}_i \) is the origin of the \( i \)th unit cell. The product is over pairs of spinors, the pairs corresponding to the up and down sublattice Cu spins in each unit cell, where, say, the up sublattice Cu site is at \( \vec{r}_i \) and then the down sublattice Cu site is at \( \vec{r}_i + \hat{x} \). The four basis sites at which the Oxygen hole may be found are denoted by \( \mu = 1, 2, 3, 4 \) (see Fig. 1), and the state of each Cu spinor can depend on which of the four sites the Oxygen hole is found at. Finally, these states are put into Bloch states labeled by some wave vector \( \vec{k} \).

The minimum energy state at each wave vector is found by minimizing the variational parameters in this wave function. The variational parameters can be understood as follows: Consider one Oxygen hole location in a lattice with \( N \) unit cells. There are \( 2N \) Cu sites implying that \( 4N \) angles fully specify the Cu spinors. Since there are four possible Oxygen hole locations per unit cell and there is a complex amplitude \( \gamma_\mu \) associated with each Oxygen position, there are a total of \( 16N + 16 \) variational parameters. However, since the absolute orientation of the spins and the overall phase of the wave function are arbitrary, there are only \( 16N + 12 \) variational parameters in this normalized wave function that are physically meaningful to change. We have numerically obtained converged results as a function of increasing \( N \).

As mentioned above, we previously found [6] that the hopping parameters that are required to make the dispersion relation of this variational wave function best approximate the ARPES data of Ref. [5], viz., \( t_a = 0.1 \) eV, \( t_b = 0.15 \) eV, and \( t_{pp} = -0.2 \) eV, are physically unreasonable — see Eq. (2). Also, the bandstructure produced from this wave function does not agree with the experimentally observed flat band from \( \vec{k} = (0, 0) \rightarrow (\pi, 0) \). Thus, we now present the formalism and motivating ideas behind our new variational wave function.

One possible reason for the failure of the three–band semiclassical wave function follows from the analysis of Zhang and Rice [3]: Quite simply, these authors showed how local hopping processes tended to quench the spin of the Oxygen hole to zero at each Oxygen site, thus producing spinless vacancies. In their formalism, this can only happen if the Oxygen hole is allowed to execute quantum fluctuations between its up and down spin states at
each site — clearly, Eq. (3) does not include the possibility of such fluctuations. Assuming that the reduction of the Oxygen hole’s spin is indeed physically important (though not necessarily conceding that this spin is quenched to zero) we introduce the following class of variational wave functions.

We have generalized the variational wave function of Ref. [8] (presented in Eq. (3)) by including Oxygen spin fluctuations. As we show below, the effect of this is to allow for quantum fluctuations of the occupied Cu–O–Cu bond, thus allowing for the quasiparticle to approximate the trion of Ref. [9]. The new variational wave function that we consider in this paper is

\[
|\Psi_{\vec{k}}\rangle = \sum_{\vec{r}} \sum_{\sigma=\uparrow,\downarrow} e^{i\vec{K}\cdot\vec{r}} \sum_{\mu=1}^{4} \gamma_{\mu,\sigma} \psi_{\mu,\sigma}^{O}(\vec{r}) \prod_{i} \psi_{\mu,\sigma}(\vec{r}_{i} - \vec{r}) \psi_{\mu,\sigma}(\vec{r}_{i} + \hat{x} - \vec{r}),
\]

(4)

where

\[
\psi_{\mu,\uparrow}^{O} = \begin{cases} 
  e^{-i\phi_{\mu}/2} \cos(\theta_{\mu}/2) \\
  e^{i\phi_{\mu}/2} \sin(\theta_{\mu}/2)
\end{cases}
\]

(5)

and

\[
\psi_{\mu,\downarrow}^{O} = \begin{cases} 
  e^{-i\phi_{\mu}/2} \sin(\theta_{\mu}/2) \\
  -e^{i\phi_{\mu}/2} \cos(\theta_{\mu}/2)
\end{cases}.
\]

(6)

The angles specifying the Cu spinors \(\psi_{\mu,\uparrow}\) and \(\psi_{\mu,\downarrow}\) for the same Cu site are allowed to be completely independent of one another. However, by enforcing the structure of the spinors of Eqs. (5,6) we ensure that the \(\sigma = \uparrow\) and \(\sigma = \downarrow\) components of this variational wave function are orthogonal to one another, and thus each product of spinors in this wave function is orthogonal to every other product of spinors.

Armed with this wave function we attempted to find hopping parameters that were close to those of Eq. (2) such that the measured dispersion relation agreed with that produced by this new variational wave function. Our results are shown in Fig. 2; clearly, the agreement that we find is superb. To the best of our knowledge, no other theory agrees with the ARPES data so accurately.
The energy parameters that enter Eq. (1) that correspond to our fitted $E \text{ vs. } \vec{k}$ data are

$$J_{\text{Cu-Cu}} = 0.125 \text{ eV}, J_{\text{Cu-O}} = 0.63 \text{ eV}, t_a = 0.25 \text{ eV}, t_b = 0.3 \text{ eV}, \text{ and } t_{pp} = -0.3 \text{ eV}.$$  

(7)

The comparison between the fitted hopping parameter values that we find and those obtained from perturbation theory/electronic structure work, viz. Eq. (2), is very pleasing except for the direct Oxygen–Oxygen hopping ($t_{pp}$) — we find a value which is about half of that predicted using other techniques. It is possible that the 10 % larger lattice constant of Sr$_2$CuO$_2$Cl$_2$ in comparison to that used in the electronic structure work is responsible for part of this difference.

In Fig. 2 we have also shown a solid curve which is a fit to the energies obtained from our variational wave function. The fit was done using

$$E(\vec{k}) = \sum_{m,n} A_{(m,n)} \cos^m(k_x) \cos^n(k_y),$$

(8)

where $A_{(m,n)} = A_{(n,m)}$ and $m + n = 2N$ ($N$ is an integer). Only terms up to and including $N = 4$ have been included in the calculation of this curve. It is clear that Eq. (8) preserves the AFM symmetry ($E(\vec{k}) = E(\vec{k} + (\pm \pi, \pm \pi))$) and also the reflections and rotations of the $C_{4v}$ point group. The coefficients that produce this curve are listed in Table I.

4. PROPERTIES OF THE VARIATIONAL WAVE FUNCTION

In this section we discuss the properties of the variational wave functions that were produced from fits to the ARPES data, and focus on two issues: (i) If the one–band $t - t' - J$ model does not lead to a fit with ARPES whereas the three–band model does, what’s the problem with the one–band model? Here we display results showing that the spin of the Oxygen hole is not quenched to zero, and thus the mobile carrier does not have a spin that is quenched to zero as it is (by definition) for the spinless vacancies of the one–band $t - t' - J$ model. (ii) If the three–band to one–band (spinless vacancy) renormalization is not adequate for all wave vectors in the first Brillouin zone, then Zhang–Rice quasiparticles
are not a good description of the carriers everywhere in the first Brillouin zone — so, what is a good description of the quasiparticles? Here we display our quantitative data verifying that the trion quasiparticle of Ref. [9] is an excellent representation of mobile carriers.

To indirectly evaluate the validity of the one–band model in describing the quasiparticles propagating in Sr$_2$CuO$_2$Cl$_2$, we have determined the magnitude of the spin of the Oxygen hole as a function of wave vector using the variational wave functions determined in the last section. To this end, we have computed the expectation value of the Oxygen spin operator:

$$\langle \vec{S}^O(\vec{k}) \rangle = \sum_{\mu} \langle \Psi_{\vec{k}} | \hat{\vec{S}}^O_{\mu} | \Psi_{\vec{k}} \rangle,$$  \hspace{1cm} (9)

where the sum over $\mu$ refers to the four Oxygen basis sites. Our results for the magnitude of the quantity defined in Eq. (9) are shown in Fig. 3. We see that along the AFM Brillouin zone the Oxygen hole’s spin is essentially quenched to zero and thus we would expect the one–band model to be a good representation of the quasiparticles along the AFM Brillouin zone — the one–band $t - t' - J$ model of Ref. [6] indeed agrees with the ARPES data along this branch. However, along the other high–symmetry branches of the first Brillouin zone we find that the spin of the Oxygen hole is not quenched to zero and is in fact quite large. Concomitantly, it is along $(0, 0) \rightarrow (\pi, 0)$ that the one–band $t - t' - J$ model has difficulties fitting the ARPES data. Thus, if these three–band variational wave functions are indeed a good representation of the true wave functions of this system, any renormalization that attempts to quench this spin and describe the motion in terms of spinless vacancies is not necessarily justified and not necessarily going to work.

If the spin of the carrier is not quenched to zero, then the spinless vacancy quasiparticles which are the biproduct of the Zhang–Rice renormalization [3] cannot be adequate. The question then remains: what is the best representation of the quasiparticles? An answer first put forward by Emery and Reiter, viz. so–called trions, can best be understood by considering the case of a single Oxygen hole localized on a Cu–O–Cu bond. From Eq. (1) we have that the Hamiltonian for this bond is nothing more than

$$H = J_{Cu-O} \vec{S}^O \cdot (\vec{S}_1 + \vec{S}_2)$$  \hspace{1cm} (10)
where $\vec{S}_1$ and $\vec{S}_2$ are the respective spins of the two Cu spins that are neighbours to the Oxygen hole. Letting the components of each ket refer to a Cu$_1$-O-Cu$_2$ labeling of the sites, the ground state of this problem is a doublet, with the $S_{\text{Total}}^z = 1/2$ wave function being given by

$$|\Psi_{g,\uparrow}\rangle = \frac{1}{\sqrt{6}} \left( 2|\uparrow,\downarrow,\uparrow\rangle - |\uparrow,\uparrow,\downarrow\rangle - |\downarrow,\uparrow,\uparrow\rangle \right).$$

(11)

Emery and Reiter [9] surmised that this and its time–reversed state were the quasiparticles, so–called trions, that moved through the lattice when the Oxygen hole was delocalized. In fact, if the spin distortions of the AFM background were prohibited (unlike our Eq. (4)), these quasiparticles were found by Klein and Aharony [16] to best describe carrier motion in CuO$_2$ planes.

As discussed in Ref. [8], an excellent representation of the true ground state of this Hamiltonian follows from a 3–spin version of the variational wave function given in Eq. (4) of this paper. In fact, the success of this kind of problem in solving the above Hamiltonian was one of the motivations for our consideration of Eq. (4) — to be specific, if we could ably represent the trions and they were indeed the appropriate quasiparticles of the mobile hole problem, these should be excellent variational wave functions. We formed the density matrix for the possible states of the occupied Cu–O–Cu bond and calculated the trion occupation for our variational wave functions found from fitting to the ARPES data; our results are shown in Fig. 4. Independent of the wave vector we find that our wave functions have an occupation of at least 92 % in the trion states. Note that for the high symmetry wave vectors the occupation is between 97 per cent and 98 per cent. Therefore, we find that the trion doublet state is an excellent representation of the quasiparticle for these planes.

5. DISCUSSION

We have presented our formalism for the extension of the Shraiman–Siggia semiclassical variational wave functions to the strong–coupling three-band model including the quantum
fluctuations of the occupied Cu-O-Cu bond. For reasonable hopping parameters we find
superb agreement with the $E$ vs. $\vec{k}$ dispersion relation that is measured experimentally in
antiferromagnetically aligned $\text{Sr}_2\text{CuO}_2\text{Cl}_2$. Since it was found that the single–band $t-t'-J$
model was not able to fit the quasiparticle dispersion throughout the entire first Brillouin
zone, perhaps the three-band model discussed in this paper will be necessary to describe the
normal–state properties of these planes. However, we can not determine the full spectral
function using this approach, and thus a more complete comparison of the measured $A(\vec{k}, \omega)$
to our three-band model is still lacking.

Theories of related spectral functions do indeed exist, but are unfortunately inadequate
to treat the task at hand: One of the most popular analytical theories of the $t-J$ model
is the self–consistent Born approximation (SCBA) $[17, 19]$. It was argued in Ref. $[13]$
that vertex corrections of the so–called spin polaron model version of the $t-J$ model were absent
(viz, those of the two–loop crossing diagram) to second–order in perturbation theory, and
thus it was expected that this theory should be very successful. This forecast was indeed
verified in a recent exact, unbiased numerical determination of the spectral function for a
single hole propagating in the largest square cluster yet doped, viz. a 32–site cluster, as
described by the $t-J$ model $[20]$ — the comparison of the exact $E$ vs. $\vec{k}$ dispersion relation
to that predicted by the SCBA led to an impressive agreement.

Unfortunately, if one includes either a next–nearest–neighbour hopping $t'$ in the one–band
model, or applies this same formalism to the three-band model $[21]$, the same cancellation of
low–order vertex corrections does not occur. Consequently, such approximate theories are
much more speculative. Thus, vertex corrections must be examined and understood before
an analytical theory of the spectral function is available, and only when it is available will a
full comparison of the spectral function of Eq. (1) to that of the experimental data of Ref.
$[5]$ be possible.

These new wave functions, and the associated $E$ vs. $\vec{k}$ dispersion relation, can be applied
to the calculation of quantities such as the Pauli susceptibility and specific heat using the
rigid–band approximation — these results will be presented in a planned future publication.
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Figure Captions

1. A schematic of the two Cu $d_{x^2-y^2}$ and four Oxygen $p_x/p_y$ orbitals of the primitive unit cell of a state with broken AFM symmetry.

2. Quasiparticle energies (solid diamonds) of an Oxygen hole in the effective Hamiltonian of Eq. (1) for an infinite lattice using our new variational wave function that includes the spin fluctuations of the Oxygen carriers. The quasiparticle dispersion measured in Ref. [5] is also shown (open circles). The parameters that produce this quasiparticle dispersion are $J_{Cu-Cu} = 0.125$ eV, $J_{Cu-O} = 0.63$ eV, $t_a = 0.25$ eV, $t_b = 0.3$ eV, and $t_{pp} = -0.3$ eV.

3. The magnitude of the Oxygen spin operator’s expectation value (solid diamonds) for a single Oxygen hole on an infinite lattice (c.f. Eq. (9)).

4. The percentage occupation of the spin–up and spin–down trion doublet states in our variational wave functions as a function of wave vector.
TABLE I. Coefficients appearing in Eq. (8) that describes the $E \text{ vs. } \vec{k}$ relation predicted by our variational wave function for the parameters of Eq. (7).

| $i$ | $j$ | $A_{ij}$ (eV) |
|-----|-----|--------------|
| 2   | 0   | 0.1755       |
| 1   | 1   | 0.03078      |
| 4   | 0   | 0.6628       |
| 3   | 1   | 0.1520       |
| 2   | 2   | 0.2694       |
| 6   | 0   | -0.7557      |
| 5   | 1   | -0.3868      |
| 4   | 2   | -0.7220      |
| 3   | 3   | -0.1955      |
| 8   | 0   | 0.2190       |
| 7   | 1   | 0.1484       |
| 6   | 2   | 0.3315       |
| 5   | 3   | 0.1420       |
| 4   | 4   | 0.2246       |
\[ \mu = 3 \]

\[ \mu = 2 \]

\[ \mu = 1 \]

\[ \mu = 4 \]
