An effective 1-band model for the cuprate superconductors

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Starting from the copper-oxygen Hamiltonian of the CuO$_2$ planes, we derive analytically an extended 1-band Hubbard Hamiltonian for the electrons on copper sites, through a canonical transformation which eliminates the oxygen sites. The model sustains a variety of phases: checkerboard states, stripes, antiferromagnetism, local pairs and mixtures thereof. This approach may be helpful in understanding what is so special about the CuO$_2$ planes, as opposed to other compounds.

I. INTRODUCTION

The starting point is the 3-band Hamiltonian, in which Cu 3$d_{x^2-y^2}$ and O 2$p_{x,y}$ orbitals are taken into account [1],

$$H_o = \sum_{i,\sigma} \epsilon_i d_{i,\sigma}^\dagger d_{i,\sigma} + \sum_{i,j,\sigma} t_{oi j} d_{i,\sigma}^\dagger d_{j,\sigma} + \sum_{i} U_i d_{i,\uparrow}^\dagger d_{i,\uparrow} d_{i,\downarrow}^\dagger d_{i,\downarrow} + \sum_{i<j,\sigma,\sigma'} V_{ij} d_{i,\sigma}^\dagger d_{i,\sigma} d_{j,\sigma'}^\dagger d_{j,\sigma'} .$$

(1)

The problem of reducing the 3-band Hamiltonian to a more amenable effective 1-band Hamiltonian has been treated in a number of papers [2, 3, 4, 5, 6, 7, 8, 9, 10]. Our goal is similar in spirit. As the holes tend to reside mostly on the Cu atoms, we wish to incorporate in the new effective Cu 1-band Hamiltonian explicit 2-particle correlations, stemming from the original Hamiltonian.

We emphasize that our approach is not a large-$U$ type (which was shown to be problematic [11]), thus allowing for double occupancy of the Cu sites. It merely eliminates the oxygen sites. To this end, we use the canonical transformation method of Chao, Spalek and Oles (CSO) [12], adapted to the Hamiltonian of eq. (1) for the CuO$_2$ planes. Besides their different Hamiltonian, ZO followed a different strategy. The transformed Hamiltonian was separated into parts depending on the number of doubly occupied sites, and oxygen sites explicitly appeared therein, in contrast to our approach.

It is understood that the present method can also be applied to lattices other than the CuO$_2$ plane.

In the following, section II contains the canonical transformation formalism. In section III we present the new transformed Hamiltonian was separated into parts depending on the number of doubly occupied sites, and oxygen sites explicitly appeared therein, in contrast to our approach.

II. CANONICAL TRANSFORMATION FORMALISM

Following CSO [12], we write the Hamiltonian as

$$H_o = H_A + H_B ,$$

(2)

$$H_B = \sum_{i,j,\sigma} t_{oi j} d_{i,\sigma}^\dagger d_{j,\sigma} = \sum_{i\neq j} P_i H_o P_j ,$$

$$H_A = H_o - H_B = \sum_{i} P_i H_o P_i ,$$

with $P_i$ being projector operators with $\sum_{j} P_j = 1$. $P_i$ projects a state on the eigenstate with eigenenergy $E_i$ of the interacting part of $H_o$, i.e. $H_A|i > = E_i |i >$. Moreover, following CSO (c.f. before eq. (6a) of ref. [12]), we assume that

$$< i | H_B | j > = 0 ,$$

$$E_i = E_j ,$$

(3)

i.e. $H_B$ does not connect states which are energetically degenerate. This condition is further discussed below.
We consider the canonical transformation

\[ H = e^{-iS} (H_A + H_B) e^{iS} \]  

\[ = H_A + H_B - i [S, H_A] + \sum_{n=2}^{\infty} \frac{(n-1)(-i)^{n-1}}{n!} [S, H_B]_{n-1} \]

where the operator \( S \) is such that

\[ H_B - i [S, H_A] = 0 \]  

This condition amounts to the elimination of the O sites from \( H \). However, the matrix elements of \( H \) between non-degenerate states depend implicitly on the occupation of the O sites - c.f. below. We use the notation

\[ [[A, B]]_n = [A, [A, [... [A, B]...]]] \]

with \( n \) commutators at the right-hand side.

Substituting eq. (5) into (4) yields

\[ H = H_A + \sum_{n=2}^{\infty} \frac{(n-1)(-i)^{n-1}}{n!} [S, H_B]_{n-1} \]

An expression for \( S \) is derived by substituting into (5) \( H_A \) and \( H_B \) from (2), and then apply the projectors \( P_j \) from the left and \( P_k \) from the right on both sides of (5), thus yielding

\[ P_j H_A P_k (1 - \delta_{jk}) + i P_j H_o P_j (P_j S P_k) - i (P_j S P_k) P_k H_A P_j = 0 \]

Noting that \( X_k = P_k H_A P_k = P_k H_A P_k \), \( X_k \) are replaced by the proper energy eigenvalues \( E_k \). For \( E_j \neq E_k \) eq. (9) leads to

\[ P_j S P_k = \frac{i P_j H_B P_k}{E_j - E_k} \]

It also follows that \( P_j S P_j = c P_j \), with \( c \) an arbitrary constant, whose value is irrelevant. Then, using eqs. (9), (10) and \( \sum_j P_j = 1 \),

\[ [[S, H_B]]_n = \left[ \left( \sum_{j \neq k} P_j S P_k, -i \sum_{l \neq m} (E_l - E_m) P_l S P_m \right) \right]_n \]

\[ = i(-1)^{n-1} \sum_{k \neq k} \left\{ \sum_{j=0}^{n} \frac{(-1)^j (n+1) j!}{j! \Gamma(n+1-j)} \right\} P_{k_1} S P_{k_2} S ... S P_{k_{n+1}} \]

and the double primed summation is restricted to \( E_{k_m} \neq E_{k_{m+1}} \) for all \( m \), in accordance with condition (5) above. Substituting \( [[S, H_B]]_n \) into eq. (7) yields

\[ H = H_A - \sum_{n=2}^{\infty} \frac{(n-1) n!}{n!} \sum_{k \neq k} \left( \sum_{j=0}^{n} \frac{(-1)^j n!}{j! \Gamma(n+1-j)} E_{k_{j+1}} \right) P_{k_1} S P_{k_2} S ... S P_{k_{n+1}} \]

This is eq. (25) of CSO. Using eq. (9), it can also be written as

\[ H = H_A - \sum_{n=2}^{\infty} (-1)^n \sum_{k \neq k} I_n(\{k_m\}) P_{k_1} H_B P_{k_2} H_B ... H_B P_{k_{n+1}} \]

where

\[ I_n(\{k_m\}) = \frac{n-1}{n!} \sum_{j=0}^{n} \frac{(-1)^j n!}{j! \Gamma(n+1-j)} \frac{E_{k_{j+1}}}{\prod_{i=1}^{j} (E_{k_i} - E_{k_{i+1}})} \]
Expressions for the factors $I_n$ used herein are given in Appendix A.

### III. Effective Hamiltonian

Carrying out the expansion to fourth order in the hopping elements $t, t', t''$, the new Hamiltonian turns out to be

$$H = \sum_{<i,j>,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} \{ t_{1a}(1-n_{j,-\sigma})(1-n_{l,-\sigma}) + t_{1b}n_{j,-\sigma}(1-n_{l,-\sigma}) + (1-n_{j,-\sigma})n_{l,-\sigma} \} + t_{1c}(1-n_{j,-\sigma})n_{l,-\sigma} + t_{1d}n_{j,-\sigma}(1-n_{l,-\sigma}) + t_{1e}(1-n_{j,-\sigma})n_{l,-\sigma} \}

= \sum_{<i,j>,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} \{ (1-n_{i,-\sigma})(1-n_{i,-\sigma})t_{2a}(1-n_{j,-\sigma})(1-n_{l,-\sigma}) + t_{2b}n_{j,-\sigma}(1-n_{i,-\sigma}) + t_{2d}n_{i,-\sigma}(1-n_{j,-\sigma})(1-n_{l,-\sigma}) + n_{i,-\sigma}(1-n_{i,-\sigma})t_{A}(1-n_{j,-\sigma})(1-n_{j,-\sigma}) + t_{B}[n_{i,-\sigma}(1-n_{j,-\sigma}) + (1-n_{i,-\sigma})n_{j,-\sigma}] + t_{C}n_{i,-\sigma}n_{j,-\sigma} \}

+ n_{i,-\sigma}n_{j,-\sigma}t_{D}(1-n_{l,-\sigma})(1-n_{l,-\sigma}) + t_{E}[n_{i,-\sigma}(1-n_{l,-\sigma}) + (1-n_{i,-\sigma})n_{l,-\sigma}] + t_{F}n_{i,-\sigma}n_{l,-\sigma} \}

- \sum_{<i,j>,\sigma} \{ A_{SXb} n_{j,-\sigma}n_{j,-\sigma}[n_{l,-\sigma}(1-n_{l,-\sigma}) + n_{l,-\sigma}(1-n_{l,-\sigma})] + A_{SXc} n_{j,-\sigma}(1-n_{l,-\sigma})(1-n_{l,-\sigma}) \}

- A_{PT} \sum_{<i,j>,\sigma} c^\dagger_{i,\sigma} c_{i,-\sigma} c_{j,-\sigma} c_{j,-\sigma} - A_{XE} \sum_{<i,j>,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} c_{j,-\sigma} c_{l,-\sigma}

- \sum_{<i,j>,\sigma} \{ c^\dagger_{i,\sigma} c_{i,-\sigma} c_{j,-\sigma} c_{l,-\sigma} + c^\dagger_{j,\sigma} c_{j,-\sigma} c_{l,-\sigma} \}

\{ A_{FBa} (1-n_{j,-\sigma})(1-n_{l,-\sigma}) + A_{FBB} [n_{j,-\sigma}(1-n_{i,-\sigma}) + (1-n_{i,-\sigma})n_{j,-\sigma}] + A_{FBC} n_{j,-\sigma}n_{i,-\sigma} \}

- \sum_{<i,j>,\sigma} c^\dagger_{i,-\sigma} c_{i,-\sigma} c_{j,-\sigma} c_{l,-\sigma} \{ A_{CMa}(1-n_{i,-\sigma})(1-n_{j,-\sigma}) + A_{CMb}(1-n_{i,-\sigma})n_{j,-\sigma}

+ A_{CMc}n_{i,-\sigma}(1-n_{j,-\sigma}) + A_{CMd}n_{i,-\sigma}n_{j,-\sigma} \}.

The indices $i, j, l$ run exclusively over the Cu lattice and $n_{i,-\sigma} = c^\dagger_{i,\sigma} c_{i,-\sigma}$. $<j,l>$ implies that $j$ and $l$ are nearest neighbors (n.n.), $<j,l;i>$ implies that $j$ and $l$ are second nearest neighbors and $i$ is the common n.n. and $<j,l;i'>$ implies that in addition to second neighbors $j$ and $l$ can be third neighbors with $i$ the middle common n.n. The term ‘empty lattice’ below refers to the case of no other electrons present than the ones hopping between initial and final positions; we ignore the electrons in the rest of the lattice. Henceforth $\epsilon = \epsilon_p - \epsilon_d$ and $V' = 0$.

We see that the only term remaining intact from the original $H_p$ is the Hubbard term on Cu sites. All hopping terms now depend on the site occupancy. The other new terms generated include superexchange (SX), a pair-transfer (PT) between n.n., an exchange of electrons (XE) between n.n., a local pair-formation or pair-breaking (FB), and a correlated motion (CM) of two electrons. The respective matrix elements are given below.

### Hopping Elements

1st neighbors - all the terms of order $t^4$ below contain a hopping forth and back between a Cu and an O atom.

Empty lattice, i.e. no other electron is present in the Cu sites $j$ and $l$ involved

$$t_{1a} = -\frac{t^2}{\epsilon + U_p - 6V} + \frac{4t^2t'}{3} \left\{ \frac{1}{V(\epsilon + U_p - 6V)} - \frac{1}{\epsilon + U_p - 7V} \right\} \frac{2}{(\epsilon + U_p - 7V)^2} \left\{ \frac{1}{\epsilon + U_p - 6V} - \frac{1}{\epsilon + U_p - 7V} \right\}$$

$$+ \frac{3t^4}{8(\epsilon + U_p - 6V)(\epsilon + U_p - 5V)} \left\{ \frac{1}{\epsilon - U + U_p - 5V} - \frac{1}{\epsilon - U + U_p - 6V} \right\} \left\{ \frac{1}{\epsilon + U_p - 5V} - \frac{1}{\epsilon + U_p - 6V} \right\}$$

$$+ \frac{3t^4}{8(\epsilon - U + U_p - 6V)(\epsilon - U + U_p - 5V)} \left\{ \frac{1}{\epsilon + U_p - 5V} - \frac{1}{\epsilon + U_p - 6V} \right\}$$
\[ \begin{align*}
&+ \frac{3t^4}{2} \left( \frac{1}{\epsilon - U + U_p - 5V} - \frac{1}{\epsilon - U + U_p - 5V} \right) + \frac{t^2 t'^2}{8V^2} \left( \frac{1}{\epsilon - U + U_p - 6V} + \frac{1}{\epsilon + U_p - 7V} \right) \quad (18) \\
&+ \frac{2t^2 t'}{3} \left( \frac{1}{2V(\epsilon - U + U_p - 5V)} - \frac{1}{2V(\epsilon - U + U_p - 7V)} \right) + \frac{1}{\epsilon - U + U_p - 6V} \left( \frac{1}{\epsilon - U + U_p - 4V} - \frac{1}{(\epsilon - U + U_p - 5V)(\epsilon + U_p - 7V)} \right) \quad (19)
\end{align*} \]

1st neighbors - an additional \(-\sigma\) electron at the initial site \(j\) or final site \(l\)

\[ t_{1b} = \frac{t^2}{2} \left( \frac{1}{\epsilon - U + U_p - 5V} - \frac{1}{\epsilon - U + U_p - 5V} \right) + \frac{t^2 t'^2}{8V^2} \left( \frac{1}{\epsilon - U + U_p - 6V} + \frac{1}{\epsilon + U_p - 7V} \right) \]

1st neighbors - an additional \(-\sigma\) electron at both initial and final sites \(j\) and \(l\)

\[ t_{1c} = -\frac{t^2}{\epsilon - U + U_p - 4V} - \frac{3t^2 t'^2}{8} \left( \frac{1}{V^2(\epsilon - U + U_p - 6V)} - \frac{2}{V(\epsilon - U + U_p - 6V)^2} \right) + \frac{2t^2 t'}{3} \left( -\frac{1}{2V(\epsilon - U + U_p - 6V)} + \frac{1}{2V(\epsilon - U + U_p - 4V)} \right) \quad (19) \\
+ \frac{1}{\epsilon - U + U_p - 4V} \left( \frac{2}{\epsilon - U + U_p - 6V} - \frac{2}{(\epsilon - U + U_p - 5V)(\epsilon + U_p - 4V)} \right) \]

1st neighbors - an additional \(-\sigma\) electron at the initial site \(j\) only

\[ t_{1d} = \frac{3t^4}{8(\epsilon - U + U_p - 4V)(\epsilon - U + U_p - 5V)} \left( \frac{1}{\epsilon + U_p - 5V} + \frac{1}{\epsilon - U + U_p - 6V} \right) + \frac{3t^4}{8(\epsilon - U + U_p - 6V)(\epsilon + U_p - 5V)} \left( \frac{3}{\epsilon - U + U_p - 4V} + \frac{4}{\epsilon - U + U_p - 5V} \right) \]

\[ + \frac{3t^4}{8(\epsilon - U + U_p - 5V)^2} \left( \frac{1}{\epsilon - U + U_p - 5V} - \frac{5}{\epsilon + U_p - 5V} \right) + \frac{3t^4}{8(\epsilon - U + U_p - 4V)(\epsilon + U_p - 7V)} \left( \frac{1}{\epsilon - U + U_p - 3V} - \frac{3}{\epsilon - U + U_p - 6V} \right) \]

\[ + \frac{3t^4}{8(\epsilon - U + U_p - 3V)(\epsilon - U + U_p - 6V)} \left( \frac{1}{\epsilon - U + U_p - 4V} - \frac{3}{\epsilon + U_p - 7V} \right) + \frac{3t^4}{4(\epsilon + U_p - 7V)(\epsilon - U + U_p - 5V)} \left( -\frac{1}{\epsilon - U + U_p - 3V} + \frac{2}{\epsilon + U_p - 5V} \right) \]
t_{1e} = \frac{t^4}{4(\epsilon - U + U_p - 5V)^2} \left \{ \frac{2}{\epsilon - U + U_p - 5V} - \frac{7}{\epsilon + U_p - 5V} \right \} \quad \text{(21)}

+ 2(\epsilon - U + U_p - 5V)(\epsilon - U + U_p - 7V) \left \{ \frac{1}{\epsilon - U + U_p - 3V} - \frac{3}{\epsilon - U + U_p - 7V} \right \} - \frac{9t^4}{4(\epsilon - U + U_p - 5V)(\epsilon - U + U_p - 3V)(\epsilon + U_p - 7V)}

+ \frac{3t^4}{8(\epsilon - U + U_p - 6V)(\epsilon + U_p - 6V)} \left \{ \frac{1}{\epsilon - U + U_p - 5V} + \frac{3}{\epsilon + U_p - 5V} \right \} + \frac{3t^4}{8(\epsilon - U + U_p - 6V)(\epsilon + U_p - 5V)} \left \{ \frac{1}{\epsilon - U + U_p - 4V} - \frac{1}{\epsilon - U + U_p - 5V} \right \}.

\textbf{2nd/3rd neighbors} - empty lattice, i.e. no other electron is present in the Cu sites involved, j initial, i intermediate and l final

\begin{align*}
t_{2a} &= -\frac{t^4}{4} \left \{ \frac{1}{(\epsilon + U_p - 5V)^2(\epsilon + U_p - 7V)} - \frac{3}{(\epsilon + U_p - 5V)(\epsilon + U_p - 7V)^2} \right \} \\
&\quad + \frac{1}{(\epsilon + U_p - 6V)^2} \left \{ \frac{1}{\epsilon + U_p - 5V} - \frac{3}{\epsilon + U_p - 7V} \right \} - \frac{6}{(\epsilon + U_p - 6V)^3}.
\end{align*} \quad \text{(22)}

\textbf{2nd/3rd neighbors} - an additional \(-\sigma\) electron at either the initial site j or final site l

\begin{align*}
t_{2b} &= -\frac{t^4}{8(\epsilon + U_p - 7V)(\epsilon + U_p - 4V)} \left \{ \frac{1}{\epsilon + U_p - 5V} + \frac{1}{\epsilon - U + U_p - 5V} - \frac{3}{\epsilon - U + U_p - 6V} - \frac{3}{\epsilon + U_p - 6V} \right \} \\
&\quad - \frac{1}{8} \left \{ \frac{1}{\epsilon + U_p - 4V} - \frac{3}{\epsilon + U_p - 7V} \right \} \left \{ \frac{1}{(\epsilon + U_p - 5V)(\epsilon - U + U_p - 6V)} + \frac{1}{(\epsilon - U + U_p - 5V)(\epsilon + U_p - 6V)} \right \} \\
&\quad + \frac{4(\epsilon + U_p - 6V)(\epsilon - U + U_p - 6V)}{4(\epsilon + U_p - 5V)(\epsilon + U_p - 6V)} \left \{ \frac{1}{\epsilon - U + U_p - 5V} + \frac{2}{\epsilon - U + U_p - 6V} \right \}.
\end{align*} \quad \text{(23)}

\textbf{2nd/3rd neighbors} - additional \(-\sigma\) electron at both initial and final sites j and l

\begin{align*}
t_{2c} &= \frac{t^4}{4(\epsilon + U_p - 4V)^2(\epsilon - U + U_p - 6V)} - \frac{3t^4}{4(\epsilon + U_p - 4V)(\epsilon - U + U_p - 6V)^2}.
\end{align*} \quad \text{(24)}
\[
\begin{align*}
- \frac{3t^4}{2(\epsilon + U_p - 5V)^2(\epsilon - U + U_p - 5V)} + \frac{t^4}{4(\epsilon - U + U_p - 5V)(\epsilon - U + U_p - 6V)} \left\{ \frac{1}{\epsilon + U_p - 4V} - \frac{3}{\epsilon + U_p - 5V} \right\} \\
+ \frac{t^4}{4(\epsilon + U_p - 4V)(\epsilon - U + U_p - 5V)} \left\{ \frac{1}{\epsilon - U + U_p - 5V} - \frac{3}{\epsilon - U + U_p - 6V} \right\}.
\end{align*}
\]

2nd/3rd neighbors - one additional $-\sigma$ electron at all 3 sites, initial, final and intermediate
\[
t_{2d} = - \frac{t^4}{8(\epsilon + U_p - 6V)^2} \left\{ \frac{1}{\epsilon + U_p - 5V} + \frac{3}{\epsilon - U + U_p - 5V} \right\} - 2(\epsilon + U_p - 6V)(\epsilon + U_p - 5V)(\epsilon - U + U_p - 5V).
\]

2nd/3rd neighbors - one additional $\sigma$ electron at intermediate site and one additional $-\sigma$ electron at either the initial site j or final site l
\[
t_A = - \frac{t^4}{(\epsilon + U_p - 6V)^3}.
\]

2nd/3rd neighbors - one additional $\sigma$ electron at intermediate site i and two additional $-\sigma$ electrons at both initial site j and final site l
\[
t_B = - \frac{3t^4}{2(\epsilon - U + U_p - 5V)^2(\epsilon + U_p - 5V)} - \frac{t^4}{4(\epsilon + U_p - 5V)^2(\epsilon - U + U_p - 5V)}.
\]

2nd/3rd neighbors - two additional electrons at intermediate site i
\[
t_D = - \frac{3t^4}{4(\epsilon - U + U_p - 5V)^2(\epsilon + U_p - 5V)} - \frac{t^4}{4(\epsilon + U_p - 5V)^2(\epsilon - U + U_p - 5V)}.
\]

2nd/3rd neighbors - two additional electrons at intermediate site i and one additional $-\sigma$ electron at either the initial site j or final site l
\[
t_E = - \frac{t^4}{2(\epsilon + U_p - 5V)(\epsilon - U + U_p - 5V)(\epsilon - U + U_p - 4V)} - \frac{3t^4}{8(\epsilon - U + U_p - 4V)^2} \left\{ \frac{3}{\epsilon + U_p - 5V} + \frac{1}{\epsilon - U + U_p - 5V} \right\}.
\]

2nd/3rd neighbors - two additional electrons at intermediate site i and two additional $-\sigma$ electrons at both initial site j and final site l
\[
t_F = - \frac{t^4}{(\epsilon - U + U_p - 4V)^3}.
\]

2nd neighbors only - an additional $-\sigma$ electron at either the initial site j or final site l
\[
t_{2e} = \frac{t^2t'}{3} \left\{ \frac{1}{V(\epsilon - U + U_p - 6V)} - \frac{1}{V(\epsilon + U_p - 7V)} - \frac{2}{(\epsilon - U + U_p - 6V)(\epsilon + U_p - 7V)} \right\}.
\]

2nd neighbors only - one additional $-\sigma$ electron at either the initial site j or final site l and one at the intermediate site i
\[
t_{2f} = \frac{t^2t'}{3} \left\{ \frac{1}{V(\epsilon - U + U_p - 6V)} - \frac{1}{V(\epsilon - U + U_p - 5V)} + \frac{2}{(\epsilon + U_p - 6V)(\epsilon - U + U_p - 5V)} \right\}.
\]

2nd neighbors only - one additional $-\sigma$ electron at either the initial site j or final site l and two at the intermediate site i
\[
t_{2g} = \frac{t^2t'}{3} \left\{ \frac{1}{V(\epsilon + U_p - 5V)} - \frac{1}{V(\epsilon - U + U_p - 4V)} + \frac{2}{(\epsilon + U_p - 5V)(\epsilon - U + U_p - 4V)} \right\}.
\]
Other elements

Transfer of a pair to a nearest neighbor site

$$A_{PT} = \frac{t^4}{2} \left\{ \frac{1}{(\epsilon - U + U_p - 5V)^2(\epsilon + U_p - 5V) + 3(\epsilon - U + U_p - 5V)(\epsilon + U_p - 5V)^2} \right\}.$$  \hspace{1cm} (35)

Transfer of a pair to a second neighbor site is $O(t^4t^2)$.

Formation/breaking of a pair - the pair is at site $l$, no other electrons at final (pair breaking)/initial (pair formation) sites $j$ and $i$

$$A_{FBA} = \frac{t^4}{4(\epsilon + U_p - 6V)^2} \left\{ \frac{1}{(\epsilon - U + U_p - 4V)^2} \left( \frac{3}{\epsilon - U + U_p - 5V} - \frac{1}{\epsilon - U + U_p - 5V} \right) \right\}.$$  \hspace{1cm} (36)

Formation/breaking of a pair - with a minus spin electron either at site $i$ or at site $j$

$$A_{FBB} = \frac{t^4}{2} \left\{ \frac{1}{(\epsilon + U_p - 6V)^2(\epsilon - U + U_p - 4V) + (\epsilon + U_p - 6V)(\epsilon - U + U_p - 4V)^2} \right\} + \frac{t^4}{8(\epsilon - U + U_p - 3V)(\epsilon + U_p - 5V)} \left\{ \frac{1}{\epsilon - U + U_p - 4V} + \frac{1}{\epsilon + U_p - 6V} \right\}.$$  \hspace{1cm} (37)

Formation/breaking of a pair - with minus spin electrons at both sites $i$ and $j$

$$A_{FBE} = \frac{t^4}{4(\epsilon - U + U_p - 5V)^2} \left\{ \frac{1}{\epsilon - U + U_p - 5V} + \frac{5}{\epsilon + U_p - 5V} \right\}.$$  \hspace{1cm} (38)

Exchange of two electrons with opposite spin - nearest neighbor case

$$A_{XE} = \frac{t^4}{2(\epsilon + U_p - 5V)^2(\epsilon - U + U_p - 5V) + 2(\epsilon + U_p - 5V)(\epsilon - U + U_p - 5V)^2} + \frac{3t^4}{30(\epsilon - U + U_p - 6V)(\epsilon + U_p - 5V)} \left\{ \frac{1}{\epsilon + U_p - 5V} + \frac{10}{\epsilon - U + U_p - 5V} \right\}.$$  \hspace{1cm} (39)

Exchange of two electrons with opposite spin - second neighbor case = $O(t^4t^2)$.

Two electrons moving to neighboring sites - empty lattice case

$$A_{CMa} = \frac{t^4}{4U(\epsilon - U + U_p - 5V)(\epsilon + U_p - 5V) + 8(\epsilon - U + U_p - 5V)(\epsilon + U_p - 5V)^2} + \frac{3t^4}{8(\epsilon - U + U_p - 5V)^2} \left\{ \frac{1}{U} + \frac{1}{\epsilon + U_p - 5V} \right\}.$$  \hspace{1cm} (40)

Two electrons moving to neighboring sites - with a minus spin electron at site $j$

$$A_{CMb} = \frac{t^4}{8(\epsilon - U + U_p - 4V)^2} \left\{ - \frac{1}{\epsilon + U_p - 5V} + \frac{9}{\epsilon - U + U_p - 5V} \right\}.$$  \hspace{1cm} (41)
Two electrons moving to neighboring sites - with a minus spin electron at site i

\[
A_{CMc} = \frac{t^4}{8(\epsilon - U + U_p - 4V)^2} \left\{ \frac{1}{\epsilon + U_p - 5V} + \frac{3}{\epsilon - U + U_p - 5V} \right\} \quad (42)
\]

Two electrons moving to neighboring sites - with minus spin electrons at both sites i and j

\[
A_{CMd} = \frac{3t^4}{2(\epsilon - U + U_p - 4V)^3} + \frac{t^4}{4(\epsilon + U_p - 5V)^2(\epsilon - U + U_p - 5V)} + \frac{3t^4}{4(\epsilon + U_p - 5V)(\epsilon - U + U_p - 4V)^2} \quad (43)
\]

Superexchange between two Cu sites - one electron at site j and a minus spin electron at site l

\[
A_{SXa} = -\frac{t^4}{4(\epsilon - U + U_p - 5V)} \left\{ \frac{1}{(\epsilon + U_p - 5V)^2} - \frac{1}{(\epsilon - U - 3V)^2} \right\} \quad (44)
\]

Superexchange between two Cu sites - two electrons at site j and one electron at site l

\[
A_{SXb} = -\frac{t^4}{(\epsilon + U_p - 4V)^3} \quad (45)
\]

Superexchange between two Cu sites - one electron at site j only, and no electron at site l, i.e. a renormalization of the site j energy, due to site l being empty

\[
A_{SXc} = -\frac{t^4}{(\epsilon + U_p - 6V)^3} \quad (46)
\]

Typically \[\epsilon = 3.6eV, t = 1.3eV, t' = 0.65eV, U = 10.5eV, U_p = 4eV, V = 1.2eV, V' = 0\]. \quad (47)

We emphasize that higher order terms are, in principle, of similar magnitude as the terms shown. Energy level degeneracies, due to finite O-O hopping, appear in fifth order of perturbation theory, restricting the present formulation. Similar issues arose in the original work of CSO \[\text{[12]}\]. One should come up with a modified procedure, possibly including an energy diagonalization in the vicinity of the Cu atom, as in \[\text{[9]}\]. Of course it is possible that the series generated are asymptotic anyway. Then the coefficients of the terms shown can be taken as merely effective parameters.

It is interesting that for parameter values close to the "typical" ones, factors such as

\[
\epsilon + U_p - m V, \quad m = 5, 6, \quad (48)
\]

may become very small in magnitude, which yields increased values of the respective interaction amplitudes A. It turns out that some effective hopping elements increase at least equally fast in that case, so that the ratios \((A/t)_{eff}\)
are finite. However, this picture may be helpful in understanding why certain e.g. 2-particle processes are important in the CuO$_2$ planes, as opposed to other lattices with different values of the original parameters. Otherwise put, *what is so special about the CuO$_2$ planes.*

**IV. GROUND STATE OF THE HAMILTONIAN**

We can treat $H$ in the Hartree-Fock-Bogoliubov approximation, with the expectation values of four operator products given by

$$< c_i c_j c_k c_l > = d_{ij} d_{kl} - d_{ik} d_{jl} + d_{il} d_{jk},$$

(49) where $d_{ij} = < c_{i,\sigma} c_{j,\sigma} >$ are numbers. Yet another obvious approximation is the replacement of the operators $n_{i,\sigma}$ by their expectation values (else we would encounter expectation values of six, instead of four, operator products).

In order to find the ground state numerically, we minimize $H$ with a fixed total number of particles $N = \sum_i n_{i,\sigma}$. This procedure requires a highly sophisticated optimization solver, able to handle several thousands of variables, with adequate constraints on their values; overall a non-trivial task [13]. In our implementation, we only looked at non-magnetized solutions.

As a first approach, we make one further simplification, taking every fermion operator as a complex number (thus having only 4 real numbers per lattice site - c.f. below). In short, within this approach, we obtained checkerboard states with periods equal to 3 by 3 and 5 by 5 (not 4) lattice sites, stripes, pure antiferromagnetic states, local pairs and mixtures thereof. E.g. an $x - y$ anisotropic checkerboard state is a mixture with a stripe state. These were found for filling factors $n = N/V = 0.8 - 1.2$ ($V$ the system volume). The nature of the ground state is mostly determined through the values of $U$ and the effective interaction and hopping parameters, rather than the filling (of course the latter dictates the values of the original CuO$_2$ plane parameters).

For a more complete solution, we should take all $d_{ij}$ above as independent parameters. This amounts to 72 real numbers per lattice site (with symmetry effects taken into consideration), making the problem very demanding computationally. The presentation of further results is postponed for a future version of this work.

Yet another route to the ground state is through the new exact variational wavefunctions which sustain superfluidity [14].

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**APPENDIX A**

Here we give explicit expressions for the first few factors $I_n$ of eq. [15]

$$I_2 = \frac{1}{2} \left( -\frac{1}{E_{12}} + \frac{1}{E_{23}} \right),$$

(50)

$$I_3 = \frac{1}{3} \left( \frac{1}{E_{12}E_{23}} - \frac{2}{E_{12}E_{34}} + \frac{1}{E_{23}E_{34}} \right),$$

(51)

$$I_4 = \frac{1}{8} \left( \frac{1}{E_{12}E_{23}E_{34}} + \frac{3}{E_{12}E_{23}E_{45}} - \frac{3}{E_{12}E_{34}E_{45}} + \frac{1}{E_{23}E_{34}E_{45}} \right),$$

(52)

$$I_5 = \frac{1}{30} \left( \frac{1}{E_{12}E_{23}E_{34}E_{45}} - \frac{4}{E_{12}E_{23}E_{34}E_{56}} + \frac{6}{E_{12}E_{23}E_{45}E_{56}} - \frac{4}{E_{12}E_{34}E_{45}E_{56}} + \frac{1}{E_{23}E_{34}E_{45}E_{56}} \right),$$

(53)

$$I_6 = \frac{1}{144} \left( \frac{1}{E_{12}E_{23}E_{34}E_{45}E_{56}} + \frac{5}{E_{12}E_{23}E_{34}E_{45}E_{67}} - \frac{10}{E_{12}E_{23}E_{34}E_{56}E_{67}} + \frac{10}{E_{12}E_{23}E_{45}E_{56}E_{67}} \right. - \frac{5}{E_{12}E_{34}E_{45}E_{56}E_{67}} + \frac{1}{E_{23}E_{34}E_{45}E_{56}E_{67}} \right),$$

(54)

where $E_{ij} = E_{k_i} - E_{k_j}$.

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