Phase diagram of the three-band half-filled Cu-O two-leg ladder

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We determine the phase diagram of the half-filled two-leg ladder both at weak and strong coupling, taking into account the Cu $d_{x^2−y^2}$ and the O $p_x$ and $p_y$ orbitals. At weak coupling, renormalization group flows are interpreted with the use of bosonization. Two different models with and without outer oxygen orbitals are examined. For physical parameters, and in the absence of the outer oxygen orbitals, the D-Mott phase arises; a dimerized phase appears when the outer oxygen atoms are included. We show that the circulating current phase that preserves translational symmetry does not appear at weak coupling. In the opposite strong-coupling atomic limit the model is purely electrostatic and the ground states may be found by simple energy minimization. The phase diagram so obtained is compared to the weak-coupling one.

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I. INTRODUCTION

Considerable effort has been expended to explain the phase diagram of the high temperature superconductors and the associated pseudogap phenomenon within the framework of quantum critical and competing order pictures. Among the several candidates for orders that could compete with superconductivity are the “circulating current (CC) phase,”1,2 the “staggered flux (SF) phase”3,4,6 or “$d$-density wave (DDW) phase,”7,5 the “spin-Peierls phase,”5,10 “stripes”11,12 or the “quantum liquid crystal phase,”13,14 and the antiferromagnetic phase.15 The CC phase, like the SF phase, breaks time reversal symmetry and is characterized by circulating currents which produce local orbital magnetic moments. An important difference between the two, however, is that the CC phase preserves translational symmetry while the SF phase breaks it.

It is a nontrivial task to ascertain phase diagrams of strongly correlated systems in two dimensions due to the lack of accurate, systematic, nonperturbative methods. Mean-field type approximations always favor from the outset particular types of orders. Exact diagonalization is constrained by small system size. Quantum Monte-Carlo methods have the notorious fermion sign problem. On the other hand, there are reliable nonperturbative methods available in one dimension such as bosonization16,17,18 and the density matrix renormalization group (DMRG) method.19,20,21 By studying ladder systems one can take a first step toward investigating some of the theoretical ideas that have been conjectured for two-dimensional systems, while remaining in an essentially one-dimensional setting. Moreover, studies of ladder systems have been strongly stimulated by synthetic compounds with the ladder structure. For example, Sr$_2$Cu$_2$O$_{4.1}$ exhibits superconductivity upon Ca doping and the application of pressure.22

Soon after the discovery of high-temperature superconductivity, one-band models such as the Hubbard or $t$-$J$ model were suggested as the simplest microscopic systems that could capture the interesting physics of the Cu-O system.23 Indeed, most work on ladders has focused on one-band models that consider only the Cu $d$ orbital.24,25,26,27,28,29,30,31,32,33,34,35,36 However, there are a number of theoretical studies,37,38 that suggest that neither the two-dimensional Hubbard nor $t$-$J$ models have a superconducting ground state. It is also impossible to capture some other types of potential order like the CC phase within a one-band model as the circulating current pattern in the CC phase involves the O orbitals in a crucial way.39 A more complete model that incorporates these orbitals is the three band or Emery model.40,41 The three-band model takes into account both strong correlations and the hybridization of Cu and O orbitals.

Relatively little work has been done on three-band ladder models so far.39,42 In this paper we obtain phase diagrams of the half-filled Cu-O ladder both at weak coupling and at strong coupling. At weak coupling, we examine ladder systems of two different geometries: with and without outer oxygen orbitals. Renormalization group (RG) flows are interpreted with the use of bosonization followed by semiclassical energy minimization. Several gapped phases arise depending on the particular values of the parameters. Within the physically relevant region, the D-Mott phase, which upon doping has a tendency toward $d$-wave superconductivity, arises in the absence of the outer oxygen sites while a spin Peierls phase occurs when outer oxygens are added. We find that the CC phase does not appear at weak coupling in the Cu-O ladder system. At strong coupling, the model is purely electrostatic. Treating the hopping term as a weak perturbation, it is then possible to make connections between the weak and strong coupling phase diagrams.

The paper is organized as follows. In Sec. II we define the models and discuss the weak-coupling continuum limit. We present the RG flow equations in Sec. III. In Sec. IV we bosonize the Hamiltonian and the various local order parameters of interest. From these, in Sec. V.
the phase diagrams of the Cu-O ladders are established
at weak coupling. The volumes of the different phases in the high-dimensional parameter space is quantified by
means of Monte-Carlo sampling. In Sec. VII we present the
phase diagram at strong coupling and compare our
findings to those at weak coupling. Our results are sum-
marized in concluding Sec. VII. Some technical details are
relegated to the Appendix.

II. MODEL

We study half-filled Cu-O two-leg ladders with Cu
d_{x^2-y^2} and O p_x and p_y orbitals as shown in Fig. 1
We consider two different geometries: (1) the five or-

tal case with two Cu d_{x^2-y^2} orbitals (i = 1, 2), two O
p_x orbitals (i = 3, 4), and one O p_y orbital (i = 5) in a
unit cell [see Fig. 1(a)] and (2) the seven orbital case in
which in addition to the five orbitals there are also two
outer oxygen p_y orbitals (i = 6, 7) [see Fig. 1(b)]. At
half-filling, on the average, there are eight electrons in a
unit cell in the five orbital model and twelve electrons in
the seven orbital model.

The Hamiltonian we investigate in this paper is given by

\[ H = H_0 + H_I, \]

where

\[ H_0 = \sum_{x,i} \epsilon_i n_i(x) - \sum_{x,i,j,\sigma} \left[ t_{ij}^{\text{intra}} c_{i\sigma}(x) c_{j\sigma}(x) \right. \]

\[ + t_{ij}^{\text{inter}} c_{i\sigma}(x) c_{j\sigma}(x-1) + \text{h.c.} \]  

(2.2)

is the tight-binding Hamiltonian and

\[ H_I = \sum_{x,i,j} U_i n_i(x) [n_j(x) - 1] + \sum_{x,i,j} \left[ V_i^{\text{intra}} n_i(x) n_j(x) \right. \]

\[ + V_i^{\text{inter}} n_i(x) n_j(x-1) \]  

(2.3)

is the Coulomb interaction. Each site is labeled by two
integers (i, x) where “i” labels atoms within a unit cell,
and “x” identifies different cells. Operators \( c_{i\sigma}(x) \) and
\( c_{i\sigma}^\dagger(x) \), respectively, annihilate and create either Cu d
electrons (i = 1, 2) or O p electrons (i = 3, 4, 5) in the
five orbital case and i = 3, 4, 5, 6, 7 in the seven orbital
case) in xth unit cell with spin \( \sigma \) (\( \sigma = \uparrow, \downarrow \)). The
number operator \( n_i(x) = \sum_\sigma c_{i\sigma}^\dagger(x) c_{i\sigma}(x) \) counts electrons
at site (i, x).

Consider now the hopping amplitudes between neigh-
boring Cu and O sites, \( t_{ij}^{\text{intra}} \) and \( t_{ij}^{\text{inter}} \) in Eq. (2.2) for the five orbital case may
be all be taken to be positive

\[ t_{ij}^{\text{intra}} = \begin{cases} \ \ |t_{ij}^{\text{dp}}| & \text{if } (i,j) = (1,3) \text{ or } (2,4) \\ \ \ |t_{ij}^{\text{dp}}| & \text{if } (i,j) = (1,5) \text{ or } (2,5) \\ \ \ |t_{ij}^{\text{pp}}| & \text{if } (i,j) = (3,5) \text{ or } (4,5) \\ \ \ 0 & \text{otherwise} \end{cases} \]

(2.4a)

\[ t_{ij}^{\text{inter}} = \begin{cases} \ \ |t_{ij}^{\text{dp}}| & \text{if } (i,j) = (1,3) \text{ or } (2,4) \\ \ \ |t_{ij}^{\text{pp}}| & \text{if } (i,j) = (3,5) \text{ or } (4,5) \\ \ \ 0 & \text{otherwise} \end{cases} \]

(2.4b)

Hopping parameters in the seven orbital case follow a
similar pattern. The on-site energy of an electron on a
Cu or O site is given by \( \epsilon_d \) or \( \epsilon_p \) respectively. For
guidance we choose on-site energies and hopping ma-
trix elements as extracted from a density functional the-
ory (DFT) calculation for YBCO by Andersen et al.15

FIG. 1: Schematic diagrams of the Cu-O ladder. (a) The
five orbital case: There are two Cu d orbitals and three O p
orbitals in a unit cell. Hopping integrals \( t_{ij}^{\text{dp}} \) and \( t_{ij}^{\text{pp}} \) are be-
 tween Cu d and O p; \( t_{ij}^{\text{pp}} \) is the hopping between the oxy-

gens. \( U_d \) and \( U_p \) are on-site Coulomb interactions, and \( V_{dp}, V_{dp}, \)
and \( V_{pp} \) are nearest-neighbor Coulomb interactions. (b) The
seven orbital case: There are two extra outer oxygen orbitals
in a unit cell labeled 6 and 7.
The case of seven orbitals again follows a similar pattern. Hole symmetry, the Fermi velocity \( v \) at the two Fermi points differs even at half filling: \( v_2 = \mu \) and \( v_1 = k_{F2} = \pi \) at half filling, where \( k_{Fn} > 0 \) is a Fermi momentum defined by \( \epsilon_n(k_{Fn}) = \mu \) and \( \mu \) is chemical potential. However, since there is no particle-hole symmetry, the Fermi velocity \( v_{Fn} = \partial \epsilon_n / \partial k|_{k=k_{Fn}} \) at the two Fermi points differs even at half filling: \( v_{F1} \neq v_{F2} \).

The band operator \( \psi_{n\sigma}(x) \) is a linear combination of the \( c_{i\sigma}(x) \)

\[
\psi_{n\sigma}(x) = \sum_i a_{in} c_{i\sigma}(x), \tag{2.7}
\]

A. Band Structure

We first diagonalize the quadratic, noninteracting portion of the Hamiltonian \( H_0 \) to obtain the band structure of the Cu-O ladder. The band structure is shown in Fig. 2. Evident in Fig. 2 is the fact that only two bands cross the Fermi level so we can analyze both ladders along the rungs \( t_{dp} \) and along the legs \( t_{dp} \) are taken to be the same, though this is not required by symmetry.

Turning now to the Coulomb interactions, the on-site energies \( U_i \) take two different values, one for Cu atoms, the other for the O atoms

\[
U_i = \begin{cases} 
    U_d & \text{if } i = 1, 2 \\
    U_p & \text{if } i = 3, 4, 5.
\end{cases} \tag{2.5}
\]

Nearest-neighbor interactions are

\[
V_{intra} = \begin{cases} 
    V_{dp} || & \text{if } (i, j) = (1, 3) \text{ or } (2, 4) \\
    V_{dp} \perp & \text{if } (i, j) = (1, 5) \text{ or } (2, 5) \\
    V_{pp} & \text{if } (i, j) = (3, 5) \text{ or } (4, 5) \\
    0 & \text{otherwise},
\end{cases} \tag{2.6a}
\]

\[
V_{inter} = \begin{cases} 
    V_{dp} || & \text{if } (i, j) = (1, 3) \text{ or } (2, 4) \\
    V_{pp} & \text{if } (i, j) = (3, 5) \text{ or } (4, 5) \\
    0 & \text{otherwise.}
\end{cases} \tag{2.6b}
\]

The case of seven orbitals again follows a similar pattern.

The Hamiltonian has the usual \( U(1) \times SU(2) \) global charge/spin symmetry. Furthermore, it is invariant under lattice translations, time reversal, parity, and chain interchange operations. As stated above, there is no particle-hole symmetry in this system in contrast to the one-band model. Since the symmetry differs, the RG equations also differ, as discussed below in Sec. III.

\[
E (\text{eV})
\]

**FIG. 2:** Energy spectrum of the quadratic portion of the Hamiltonian in momentum space. (a) Five orbital case: Three low-lying bands are completely filled and only the upper two bands intersect the Fermi level. The Fermi velocities at \( k_{F1} \) and \( k_{F2} \) differ even at half filling unlike the one band model. We use \( \epsilon_d - \epsilon_p = 3.0 \text{ eV}, t_{dp} = 1.6 \text{ eV}, \) and \( t_{pp} = 1.1 \text{ eV} \) per the DFT calculation of Andersen et al. (see Ref. 13). (b) Seven orbital case for the same parameters as the five orbital case.

\[
|a_{1n}| = |a_{2n}|, \quad |a_{3n}| = |a_{4n}|, \quad |a_{6n}| = |a_{7n}|. \tag{2.8}
\]

where \( n = 1, 2, \ldots, 5, (6, 7) \) is a band index and \( i = 1, 2, \ldots, 5, (6, 7) \) is a site index in a unit cell. It is always possible to choose the matrix element \( a_{in} \) to be real since the Hamiltonian is time-reversal invariant. Furthermore, due to the symmetry under chain exchange, we have the following relations between \( a_{in} \):

\[
\epsilon = \epsilon_d - \epsilon_p = 3.0 \text{ eV}, \quad t_{dp} = 1.6 \text{ eV}, \quad \text{and } t_{pp} = 1.1 \text{ eV}. \]
At weak coupling it suffices to focus only on the four Fermi points. Therefore, we will consider only the upper two bands \((n = 1, 2)\) in the subsequent calculation, since the completely filled bands are not active. We linearize the bands around the Fermi points and decompose the band operators into right and left moving fermion fields \(\psi_{nR\sigma}/\psi_{nL\sigma}\):

\[
\psi_{n\sigma} \propto \psi_{nR\sigma} e^{ikF_{n}x} + \psi_{nL\sigma} e^{-ikF_{n}x}. \tag{2.9}
\]

With this decomposition \(H_{0}\) reduces to

\[
H_{0} = - \sum_{n, \sigma} \int dxF_{n} \left( \psi_{nR\sigma}^{\dagger} \partial_{x} \psi_{nR\sigma} - \psi_{nL\sigma}^{\dagger} \partial_{x} \psi_{nL\sigma} \right). \tag{2.10}
\]

### B. Interaction Hamiltonian - Current Algebra

We now discuss the interactions between the electrons around the four Fermi points. We introduce the usual current operators\textsuperscript{26,44}:

\[
J_{nP} = :\psi_{nP\alpha}^{\dagger} \psi_{nP\alpha} :; \quad J_{n\bar{\sigma}} = \mathbf{1}/2 \cdot \psi_{n\bar{\sigma}}^{\dagger} \sigma_{\alpha\bar{\beta}} \psi_{n\beta};
\]

\[
L_{P} = \psi_{1P\alpha}^{\dagger} \psi_{2P\alpha} , \quad L_{P} = \mathbf{1}/2 \psi_{1\bar{\sigma}}^{\dagger} \sigma_{\alpha\bar{\beta}} \psi_{2\beta};
\]

\[
M_{nP} = \mathbf{1}/2 \psi_{nP\alpha}^{\dagger} \sigma_{\alpha\beta} \psi_{n\beta} , \quad N_{P\alpha\beta} = \psi_{1P\alpha} \psi_{2\beta}; \tag{2.11}
\]

where \(\sigma\) denotes Pauli matrices, \(P\) denotes the chirality (\(R\) or \(L\)), and \(\mathbf{1}\) : means normal ordering (vacuum subtraction.) Normal ordering signs are suppressed in the subsequent discussion for notational convenience. We also follow the notation of Balents et al.\textsuperscript{28} to permit comparison between the RG equations for the one- and three-band ladder systems in the Sec. III.

Interaction Hamiltonian density \(\mathcal{H}_{I}\) can be expressed into three parts in terms of their nature. Let \(\mathcal{H}_{I} = \mathcal{H}_{I}^{(1)} + \mathcal{H}_{I}^{(2)} + \mathcal{H}_{I}^{(3)}\).

There are eight allowed interactions connecting left and right movers, with Hamiltonian densities \(\mathcal{H}_{I}^{(1)}:\)

\[
- \mathcal{H}_{I}^{(1)} = \bar{g}_{1\rho} J_{1\rho} J_{L} + \bar{g}_{2\rho} J_{2\rho} J_{L} + \bar{g}_{\rho}(J_{1\rho} J_{2L} + J_{2\rho} J_{1L}) + \bar{g}_{\rho} J_{2\rho} \cdot J_{L} + \bar{g}_{\rho} \cdot J_{2L} \cdot J_{L} + \bar{g}_{\rho}(J_{1\rho} \cdot J_{2L} + J_{2\rho} \cdot J_{1L}) + \bar{g}_{\rho}(L_{R} L_{L} + L_{L} L_{R}). \tag{2.12}
\]

Six additional interactions are completely chiral

\[
- \mathcal{H}_{I}^{(2)} = \lambda_{1\rho} (J_{1\rho}^{2} + J_{2L}^{2}) + \lambda_{2\rho} (J_{2\rho}^{2} + J_{1L}^{2}) + \lambda_{\rho}(J_{1\rho} J_{2L} + J_{2\rho} J_{1L}) + \lambda_{\rho}(J_{1\rho} J_{2L} + J_{2\rho} J_{1L}) + \lambda_{\rho}(J_{2\rho} J_{1\rho} J_{2L} + J_{2\rho} J_{1\rho} J_{1L}). \tag{2.13}
\]

The couplings in Eq. (2.13) just renormalize the velocities of the charge and spin modes, and can be neglected in our second order calculation. Additional \(M_{nP}\) and \(N_{P\alpha\beta}\) operators must be introduced to describe Umklapp processes

\[
- \mathcal{H}_{I}^{(3)} = \bar{g}_{1\nu}(M_{1R}^{\dagger} M_{1L} + M_{1L}^{\dagger} M_{1R}) + \bar{g}_{\nu}(M_{2R}^{\dagger} M_{2L} + M_{2L}^{\dagger} M_{2R}) + \bar{g}_{\nu}(M_{1R}^{\dagger} M_{2L} + M_{1L}^{\dagger} M_{2R}) + \bar{g}_{\nu}(M_{2R}^{\dagger} M_{1L} + M_{2L}^{\dagger} M_{1R}) + \bar{g}_{\nu}(N_{1R}^{\dagger} N_{1L} + N_{1L}^{\dagger} N_{1R}) + \bar{g}_{\nu}(N_{2R}^{\dagger} N_{2L} + N_{2L}^{\dagger} N_{2R}) \tag{2.14}
\]

At half-filling the three interband Umklapp terms \((\bar{g}_{\nu}u, \bar{g}_{\nu}u_{1}, \bar{g}_{\nu}u_{2})\) are nonvanishing. The single-band Umklapp term, \(g_{\nu}u_{n}\), is nonzero only if \(k_{\nu} = \pi/2\). The detailed relationships between \(g\) and \(U, \nu\) are listed in the Appendix.

### III. RENORMALIZATION GROUP

We employ the RG approach combined with bosonization followed by semiclassical energy minimization to obtain the phase diagram at weak coupling. Comparison of the method to results of essentially exact DMRG calculations has shown it to be qualitatively reliable in cases where agreement has been checked; see for instance Ref. 52.

The current algebra as outlined in Balents et al.\textsuperscript{28} may be used to obtain one-loop RG flow equations for coupling constants. At half-filling there are eleven coupling constants, and the full set of equations is given by

\[
\dot{g}_{1\rho} = \beta \left( g_{1\rho}^{2} + \frac{3}{16} g_{1\sigma}^{2} - g_{1\nu}^{2} - g_{1\nu} g_{1\tau} - g_{1\nu}^{2} \right),
\]

\[
\dot{g}_{2\rho} = \alpha \left( g_{2\rho}^{2} + \frac{3}{16} g_{2\sigma}^{2} - g_{2\nu}^{2} - g_{2\nu} g_{2\tau} - g_{2\nu}^{2} \right),
\]

\[
\dot{g}_{x\rho} = \alpha \left( g_{x\rho}^{2} - \frac{3}{16} g_{x\sigma}^{2} - g_{x\nu}^{2} - g_{x\nu} g_{x\tau} - g_{x\nu}^{2} - g_{x\nu}^{2} \right),
\]

\[
\dot{g}_{1\sigma} = \beta \left( 2g_{1\rho} g_{1\sigma} - \frac{1}{2} g_{1\nu}^{2} - 4g_{1\nu}^{2} - 4g_{1\nu} g_{1\tau} - g_{1\nu}^{2} \right) - \alpha g_{1\sigma}^{2},
\]

\[
\dot{g}_{2\sigma} = \alpha \left( 2g_{2\rho} g_{2\sigma} - \frac{1}{2} g_{2\nu}^{2} - 4g_{2\nu}^{2} - 4g_{2\nu} g_{2\tau} - g_{2\nu}^{2} \right) - \beta g_{2\sigma}^{2},
\]

\[
\dot{g}_{x\sigma} = \alpha \left( 2g_{x\rho} g_{x\sigma} - \frac{1}{2} g_{x\nu}^{2} - 4g_{x\nu}^{2} - 4g_{x\nu} g_{x\tau} - g_{x\nu}^{2} \right) - \beta g_{x\sigma}^{2},
\]

\[
\dot{g}_{1\tau} = g_{1\rho} g_{1\tau} + \frac{3}{16} g_{1\rho} g_{1\sigma} - g_{x\rho}(g_{x\nu} - g_{x\nu} g_{x\tau} - g_{x\nu}^{2}),
\]
\[ g_\sigma = g_\sigma^0 + \left( g_\sigma^0 - \frac{1}{2} 2 g_{x\sigma}^0 - 2 g_{x\sigma}^0 \right) g_\sigma + 4 g_{x\sigma} (g_{tu1} + g_{tu2}), \]
\[ \dot{g}_{x\sigma} = g_{x\sigma}^0 + \left( g_{x\sigma}^0 - \frac{1}{2} 2 g_{x\sigma}^0 - 2 g_{x\sigma}^0 \right) g_{x\sigma} + 4 g_{x\sigma} (g_{tu1} + g_{tu2}), \]
\[ g_{tu1} = - \left( 2 g_{x\sigma} + \frac{3}{2} g_{x\sigma} \right) g_{tu1} + \left( 2 g_{x\sigma} + \frac{3}{2} g_{x\sigma} \right) g_{tu2} \]
\[ g_{tu2} = \left( 2 g_{x\sigma} + \frac{3}{2} g_{x\sigma} \right) g_{tu1} - \left( 2 g_{x\sigma} + \frac{3}{2} g_{x\sigma} \right) g_{tu2} \]

where \( g_i \equiv \frac{g_i}{\sigma} / [\pi (F_1 + F_2)] \), \( \alpha = (F_1 + F_2)/2 F_1 \), \( \beta = (F_1 + F_2)/2 F_1 \), \( g_{x\sigma} = g_{x\sigma}^0 \), and \( g_{x\sigma} = g_{x\sigma}^0 \). The dot indicates logarithmic derivative with respect to the length scale, \( g_i \equiv \partial g_i / \partial s \), where \( s = \ln l \).

The set of RG flow equations obtained in this system is different from those obtained in one band case, due to the absence of particle-hole symmetry in Cu-O. The fermionic field operator \( \psi_{n,\sigma} \) is first expressed in terms of dual Hermitian bosonic fields \( \phi_{n,\sigma} \) and \( \theta_{n,\sigma} \) by
\[ \psi_{n,\sigma} = \frac{1}{\sqrt{2 \pi \epsilon}} \kappa_{n,\sigma} \exp \left[ i (P \phi_{n,\sigma} + \theta_{n,\sigma}) \right], \]
where \( \epsilon \) is a short-distance cutoff, and again \( P = R \) or \( L = \pm 1 \) is chirality. The bosonic fields satisfy the usual commutation relations
\[ [\phi_{n,\sigma} (x), \phi_{n',\sigma'} (x')] = [\theta_{n,\sigma} (x), \theta_{n',\sigma'} (x')] = 0, \]
\[ [\phi_{n,\sigma} (x), \theta_{n',\sigma'} (x')] = i \pi \delta_{n,n'} \delta_{\sigma,\sigma'} \Theta (x-x'), \]
where \( \Theta (x) \) is the Heaviside function. The Klein factor \( \kappa_{n,\sigma} \) is introduced to ensure the correct anticommutation relations of the original fermionic fields; \( \kappa_{n,\sigma} \) commutes with the bosonic fields, and satisfies
\[ \{ \kappa_{n,\sigma}, \kappa_{n',\sigma'} \} = 2 \delta_{n,n'} \delta_{\sigma,\sigma'}. \]

A canonical transformation separates bosons into charge and spin pieces
\[ (\phi, \theta)_{n,\rho} = \frac{1}{\sqrt{2}} [ (\phi, \theta)_{n,\uparrow} + (\phi, \theta)_{n,\downarrow} ], \]
\[ (\phi, \theta)_{n,\sigma} = \frac{1}{\sqrt{2}} [ (\phi, \theta)_{n,\uparrow} - (\phi, \theta)_{n,\downarrow} ]. \]
We also define \( (\phi, \theta)_{r,\nu} \) as the following:
\[ (\phi, \theta)_{r,\nu} = \frac{1}{\sqrt{2}} \left[ r (\phi, \theta)_{1,\uparrow} + (\phi, \theta)_{2,\nu} \right], \]
where \( r \) is either + or −. With these definitions, the noninteracting part of the Hamiltonian density has the following form:
\[ H_0 = \frac{v_F^1 + v_F^2}{2 \pi} \sum_{r,\nu} \left( \partial_x \phi_{r,\nu} \right)^2 + \left( \partial_x \theta_{r,\nu} \right)^2 \]
\[ - \frac{v_F^1 - v_F^2}{2 \pi} \sum_{r,\nu} \left( \partial_x \phi_{r,\nu} \right) (\partial_x \phi_{r,\nu}) + (\partial_x \theta_{r,\nu}) (\partial_x \theta_{r,\nu}). \]
The momentum-conserving part of the interaction can be written as the sum of two terms, \( H^{(1)}_I = H^{(1a)}_I + H^{(1b)}_I \), where
\[ H^{(1a)}_I = \frac{1}{2 \pi} \sum_{r,\nu} A_{r,\nu} \left[ (\partial_x \phi_{r,\nu})^2 - (\partial_x \theta_{r,\nu})^2 \right] \]
with
\[ A_{r,\nu} = - \frac{1}{2} [ g_{x,\rho} + g_{x,\sigma} + 2 g_{x,\sigma} ], \]
\[ A_{r,\sigma} = - \frac{1}{8} [ g_{x,\rho} + g_{x,\sigma} + 2 g_{x,\sigma} ]. \]
And
\[ H^{(1b)}_I = - \frac{1}{(2 \pi e)^2} \left[ 2 \tilde{g}_{\tau,\sigma} \cos 2 \theta_{-\rho} \cos 2 \phi_{+\sigma} - (g_{x,\rho} + g_{x,\sigma} \right] \times \cos 2 \phi_{+\sigma} \cos 2 \phi_{-\rho} - \tilde{g}_{x,\sigma} \cos 2 \phi_{+�} \cos 2 \theta_{-\sigma} \]
\[ + \cos 2 \theta_{-\rho} (\tilde{g}_{x,\sigma} \cos 2 \phi_{-\sigma} + g_{x,\sigma} \cos 2 \theta_{-\sigma} ). \]
quantum disordered phases (D-Mott, D phase, the diagonal current (DC) phase, and the four bosonic fields are as follows:

| CDW  | 0   | 0   | π/2 | 0   | *   |
| SP   | π/2 | 0   | π/2 | 0   | *   |
| SF   | 0   | 0   | 0   | 0   | *   |
| DC   | π/2 | 0   | 0   | 0   | *   |
| D-Mott | 0   | 0   | 0   | *   | 0   |
| D'-Mott | π/2 | 0   | π/2 | *   | 0   |
| S-Mott | 0   | 0   | π/2 | *   | 0   |
| S'-Mott | π/2 | 0   | π/2 | *   | 0   |

TABLE I: Potential phases of the Cu-O two-leg ladder, and their pinned configurations (a * means that the field is fluctuating.)

with $g^\pm_\nu = g_\nu \mp 4g_\nu$ and $\hat{\Gamma} = \kappa_{1}\kappa_1\kappa_{2}\kappa_{2}$. Finally, the bosonized form of the Umklapp interaction density reads

$$\mathcal{H}_{1}^{(3)} = \frac{2}{(2\pi)^{2}} \cos 2\phi_{-\rho} + 2(\hat{\Gamma} g_{u1} + g_{u2}) \cos 2\phi_{+\sigma} + \frac{2}{g_{u1}} \cos 2\phi_{-\sigma} + \hat{\Gamma} g_{u1} \cos 2\theta_{-\sigma},$$

with $g^\pm_\nu = (g_{u1} + g_{u2}) \pm 4(g_{u1} - g_{u2})$.

Note that since the Hermitian operator $\hat{\Gamma}$ obeys $\hat{\Gamma}^2 = I$, $\hat{\Gamma}$ has eigenvalues $\Gamma = \pm 1$. Furthermore, since $[H, \Gamma] = 0$, $H$ and $\Gamma$ can be simultaneously diagonalized. We choose $\Gamma = 1$ in this paper. See Refs. [26] for details regarding to the subtleties of the Klein factors. For the sake of simplicity we also suppress the Klein factors in what follows.

At half-filling the system is either fully gapped (by far the most common case) or gapless in all sectors (referred to as C2S2 – see Ref. [26].) We do not find any partially gapped phases at half-filling. For the gapless phases the ground state configuration of the bosonic fields can be determined by minimizing the energy of the low-energy effective Hamiltonian at the end of the RG flow.

Once the ground state configuration of the bosonic fields is determined, the bosonized order parameters may be examined to determine the physical nature of the ground states. We consider the same order parameters studied in previous work on one-band ladder systems: the order parameter of the $(\pi, \pi)$ charge density wave (CDW) phase, the $(\pi, \pi)$ spin Peierls (SP) phase, the SF phase, the diagonal current (DC) phase, and the four quantum disordered phases (D-Mott, D'-Mott, S-Mott, and S'-Mott.) Order parameters expressed in terms of bosonic fields are as follows:

$$\mathcal{O}_{\text{CDW}} \propto \cos \phi_{+\rho} \sin \theta_{-\rho} \cos \phi_{+\sigma} \cos \theta_{-\sigma} + \sin \phi_{+\rho} \cos \theta_{-\rho} \sin \phi_{+\sigma} \sin \theta_{-\sigma},$$

$$\mathcal{O}_{\text{SP}} \propto \cos \phi_{+\rho} \cos \theta_{-\rho} \sin \phi_{+\sigma} \sin \theta_{-\sigma} + \sin \phi_{+\rho} \sin \theta_{-\rho} \cos \phi_{+\sigma} \cos \theta_{-\sigma},$$

We emphasize that Klein factors have been taken into account in the derivation of these expressions, though we suppress the Klein factors for sake of simplicity (see Refs. [26, 30, 31] for more details.) Note that $\mathcal{O}_{\text{D-Mott}}$ is the order parameter for both D-Mott and D’-Mott phase (the same holds between S-Mott and S’-Mott.) These primed phases are half-cell translated states of the unprimed states since $\phi_{+\rho}$ differs by $\pi/2$. The bosonized form of the order parameters is essentially the same as in one band case except for the appearance of complicated band coefficients $a_{ij}$.

Note also that the order parameter of the circulating current phase that preserves translational symmetry does not appear in Eqs. (4.10). This is because the long-wavelength part of the current is determined by gradients of the boson fields, $\partial_j \theta_{+\rho}$, but these cannot acquire non-zero expectation values at the semiclassical minima. Field $\theta_{-\rho}$ locks into the particular values specified in Table II and field $\theta_{+\rho}$ fluctuates with zero mean gradient. The bosonized form of the current along any link inside the unit cell, apart from the unimportant gradient terms, is given by

$$j_{ij}(x) \propto (-1)^{x} a_{ij}(a_{11}a_{21} - a_{12}a_{21}) \times (\cos \phi_{+\rho} \cos \theta_{-\rho} \cos \phi_{+\sigma} \cos \theta_{-\sigma} + \sin \phi_{+\rho} \sin \theta_{-\rho} \sin \phi_{+\sigma} \sin \theta_{-\sigma}).$$

It is clear from this expression that the current pattern, if it exists, must be staggered along the leg direction such that it breaks translational symmetry. Hence, the circulating current phase cannot occur at weak coupling in half-filled Cu-O two-leg ladder system. Furthermore, this is also true away from half-filling, at least as long as the Fermi level intersects only two bands.
We sample the parameter space determined by Monte-Carlo sampling in the five orbital case. We find that the D-Mott, S-Mott, and CDW phases occupy most of the parameter space. The volume of each phase over the entire parameter space at random, we may quantify the volume of the D-Mott or the SF phase is not possible since two bosonic fields simultaneously: \( \theta_{-\rho} \) and \( \phi_{-\sigma} \) or \( \theta_{-\rho} \) (In the one-band model, for example, the SF phase mediates the transition between the D-Mott and the CDW phase). The SF phase arises next to the D-Mott phase in the fourth quadrant bisecting the D-Mott phase. A tiny portion of the D-Mott phase exists between the D-Mott and the SF phases, which can be understood with the same argument used for the transition between the D-Mott and the CDW: a direct transition from the S-Mott to the D-Mott or the SF phase is not possible since two bosonic fields must become unpinned simultaneously. Increasing \( V_{pp} \) and holding other parameters fixed, the SF phase shrinks and then vanishes. Except for the disappearance of the SF phase, the phase diagram is qualitatively similar to Fig. 3 with slightly different phase boundaries.

The phase diagram of the seven orbital case is presented in Fig. 4. The phase diagram is topologically rather similar to the five orbital case, however, with two notable differences: the SP phase now appears inside the D-Mott phase, and the SF phase disappears altogether. Both of these aspects might be related to the anisotropy between the effective exchange integrals parallel and perpendicular to the legs. In a DMRG calculation on a two-leg Cu-O ladder system by Nishimoto et al., it was found that in the absence of the outer O orbitals, the dimensionless anisotropy ratio \( R = \langle S_i \cdot S_j \rangle_{\text{rung}} / \langle S_i \cdot S_j \rangle_{\text{leg}} \) becomes significantly larger than one. Nishimoto et al. concluded that the inclusion of outer oxygens is crucial for a qualitatively correct description of two-leg Cu-O ladders. We can understand this behavior as follows. When \( R \) is smaller and the system is therefore more isotropic, the SP phase seems to be a more stable state than the D-Mott phase, as the D-Mott phase may be thought of as a product of rung singlets. For large values of the anisotropy ratio, the strong effective Heisenberg interaction along the rung makes rung singlets relatively strong, favoring the D-Mott phase.
and in the seven orbital case

\[ J^\parallel = J^\perp = \frac{4t_{dp}^4}{(\epsilon + U_d - U_p + 7V_{dp} - 8V_{pp})^2} \times \left( \frac{1}{U_d} + \frac{2}{2\epsilon + 2U_d - U_p + 4V_{dp} - 16V_{pp}} \right) \]

\[ (6.2) \]

where the on-site energy difference between the \( d \) and \( p \) electrons is \( \epsilon = \epsilon_d - \epsilon_p > 0 \). With these effective superexchange interactions, degeneracies in the spin degree of freedom are lifted with antiferromagnetic interactions appearing when \( U_d > U_p > 0 \) and \( V_{dp} > V_{pp} > 0 \). It is easy to see that the anisotropy ratio is larger than one in five orbital case within this simple calculation, qualitatively consistent with the previous DMRG calculation. This phase can then be mapped to the D-Mott phase found at weak coupling in a similar region of parameter space. In the seven orbital case, the exchanges are isotropic, weakening tendencies towards a D-Mott phase. It should be noted, however, that if we set \( V_{pp} = 0 \) in the five orbital case, the system becomes isotropic \( J^\parallel = J^\perp \) but the SP phase still does not arise. Another possible way to explain the SP phase is to consider frustration. For example, competition between spin exchange along the plaquette and along the diagonal can stabilize the SP phase. Also, as pointed out by Kivelson et al., other higher order interactions such as plaquette four-spin ring exchange interaction can be comparable in magnitude to the superexchange energy even at relatively large \( U \), and other phases may arise due to the competition between superexchange and ring exchange interactions.

For \( U < 0 \), the \((\pi, \pi)\) CDW phase arises in a similar region as that found in the case of weak coupling. It is robust against perturbation due to the hopping term. We also find other charge ordered phases that have no direct relationship to the weak coupling phase diagram. All of these charge ordered phases have tendencies toward stripes or charge separation. Phase S1, near the negative \( U \) axis with positive \( V \), has two holes occupying the \( O p_y \) orbital. The ladder breaks into two decoupled completely filled chains. In the S2 regime, two holes occupy \( O p_x \) orbitals on a leg in doubled unit cell. In the S3 regime, pairs of two holes occupy the \( Cu \) orbital and the \( O p_x \) orbitals on a leg in doubled unit cell. In S4 and S5, holes gather around a \( Cu \) site. Finally, in the S6 regime holes gather along one leg of the ladder, and the other leg is completely filled.

\section{VII. CONCLUSION}

We determined the phase diagram of the half-filled \( Cu-O \) two-leg ladder both at weak and strong coupling. At weak coupling, perturbative RG flows are interpreted with the use of bosonization. Due to absence of particle-hole symmetry the Fermi velocities of the two bands differ to each other and different RG flow equations govern the three band model than in the case of the simple one-band ladder. After bosonization, however, the
Hamiltonian and the order parameters have essentially the same form as in the one-band case; it is the phase diagrams that differ qualitatively. By studying the Cu-O ladder with and without outer oxygen sites, four interesting conclusions may be drawn. First, in the physically relevant regime, the D-Mott phase arises when outer oxygen sites are absent. Second, the SP phase appears in the seven orbital case. Third, the SF phase only appears when the outer oxygen sites are absent. The appearance/disappearance of phases may be related to the anisotropy of the effective exchange energies in the system. Finally, we found that the CC phase which preserves lattice translational symmetry does not appear, at least at weak coupling in the Cu-O two-leg ladder. Local currents or charge modulation, when they arise, always have a staggered pattern.

VIII. ACKNOWLEDGMENTS

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APPENDIX: RELATION BETWEEN THE CONTINUUM COUPLINGS AND THE LATTICE MODEL INTERACTION PARAMETERS

In this appendix we discuss the relations between the continuum coupling constants \( \lambda \) and \( g \) and the lattice Coulomb interactions \( U \) and \( V \). Define \( w_{ij}^{(0)} \) and \( w_{ij}^{(1)} \) as follows:

\[
\begin{align*}
    w_{ij}^{(0)} &= U_{ij} \delta_{ij} + V_{ij}^{\text{intra}}, \quad \text{(A.1a)} \\
    w_{ij}^{(1)} &= V_{ij}^{\text{inter}}, \quad \text{(A.1b)}
\end{align*}
\]

where \( U_{ij}, V_{ij}^{\text{intra}}, \) and \( V_{ij}^{\text{inter}} \) are given in Eqs. (2.15) and (2.16). Parameters \( w_{ij}^{(0)} \) and \( w_{ij}^{(1)} \) represent the intracell and intercell interactions, respectively. Double-counting is avoided by taking \( w_{ij}^{(q)} \) to not be symmetric. We introduce coefficients \( f(i,j,k,l,m,n,p,q) \) as

\[
\begin{align*}
    f(i,j,k,l,m,n,p,q) &= -a_{ik}a_{kl}a_{jn} \cos((kF_{lm} + pkF_{n})q)w_{ij}^{(q)}, \quad \text{(A.2)}
\end{align*}
\]

where \( i \) and \( j \) are site indices, \( k, l, m, \) and \( n \) are band indices, \( p = \pm 1, \) and \( q = 0, 1. \)

With these definitions, the continuum coupling constants \( \tilde{\lambda} \) and \( \tilde{g} \) are given by

\[
\begin{align*}
    \tilde{\lambda}_{1\rho} &= \sum_{i,j,q} f(i,j,1,1,1,1,-1,q), \\
    \tilde{\lambda}_{2\rho} &= \sum_{i,j,q} f(i,j,1,2,2,2,1,q), \\
    \tilde{\lambda}_{x\rho} &= \sum_{i,j,q} f(i,j,1,1,2,2,1,1,-1,q) + f(i,j,1,2,2,1,1,-1,q) \\
    &- f(i,j,1,2,2,1,1,q),
\end{align*}
\]

\[
\begin{align*}
    \tilde{\lambda}_{1\sigma} &= \tilde{\lambda}_{2\sigma} = 0, \\
    \tilde{\lambda}_{x\sigma} &= -4 \sum_{i,j,q} f(i,j,1,2,2,1,-1,q), \\
    \tilde{g}_{1\rho} &= \sum_{i,j,q} 2f(i,j,1,1,1,1,-1,q) - f(i,j,1,1,1,1,1,q), \\
    \tilde{g}_{2\rho} &= \sum_{i,j,q} 2f(i,j,2,2,2,2,1,q) - f(i,j,2,2,2,2,1,1,q), \\
    \tilde{g}_{x\rho} &= \sum_{i,j,q} f(i,j,1,1,2,2,1,1,-1,q) + f(i,j,2,2,1,1,1,q) \\
    &- f(i,j,1,2,2,1,1,q),
\end{align*}
\]

\[
\begin{align*}
    \tilde{g}_{1\sigma} &= -4 \sum_{i,j,q} f(i,j,1,1,1,1,q), \\
    \tilde{g}_{2\sigma} &= -4 \sum_{i,j,q} f(i,j,2,2,2,1,q), \\
    \tilde{g}_{x\sigma} &= -4 \sum_{i,j,q} f(i,j,1,2,2,1,1,q), \\
    \tilde{g}_{\mu\rho} &= \sum_{i,j,q} 2f(i,j,1,2,2,1,2,1,q) - f(i,j,1,2,1,2,1,1,q), \\
    \tilde{g}_{\nu\rho} &= -4 \sum_{i,j,q} f(i,j,1,2,1,2,1,q), \\
    \tilde{g}_{\mu\sigma} &= \sum_{i,j,q} 2f(i,j,1,2,1,2,1,q).
\end{align*}
\]
The sum in each of the above equations runs over all site indices in the unit cell. Equations (A.3) are the most general form of coupling constants for the case of two bands cutting the Fermi level and short range Coulomb interactions. By modifying $w^{(0)}$ or $w^{(1)}$ further generalizations can be studied.

\[ \tilde{g}_{\text{tuv}} = \sum_{i,j,q} f(i, j, 1, 1, 2, 2, 1, q) + f(i, j, 2, 2, 1, 1, q), \]
\[ \tilde{g}_{\text{tuv}} = -2 \sum_{i,j,q} f(i, j, 1, 2, 2, 1, q). \]