Absence of Luther-Emery Superconducting Phase in the Three-Band Model for Cuprate Ladders

Jeong-Pil Song and Sumit Mazumdar
Department of Physics, The University of Arizona Tucson, AZ 85721

R. Torsten Clay
Department of Physics & Astronomy, and HPC² Center for Computational Sciences, Mississippi State University, Mississippi State, MS 39762
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Correlated-electron theories of superconductivity in layered cuprates often start from the premise of a gapped spin-liquid phase proximate to the superconducting state. This assumption is justified based on analytical and numerical demonstrations of a superconducting Luther-Emery phase in the doped 2-leg one-band Hubbard ladder, and the perceived analogy between coupled ladders and the two dimensional CuO

layer. We demonstrate from accurate density matrix renormalization group studies the absence of the superconducting Luther-Emery phase in the doped 2-leg three-band ladder consisting of both copper and oxygen, even as the spin gap is large in the undoped three-band ladder. For realistic oxygen-oxygen hopping and Hubbard repulsion on the oxygen atoms, density-density rather than pairing correlations are dominant at long range. This result is equally valid whether or not the oxygens outside the ladder proper, over and above the rung and leg oxygens, are included in the computation. These results demonstrate the critical importance of oxygen orbitals, and raise disturbing questions about the applicability of many of the existing correlated-electron theories of superconductivity.

I. INTRODUCTION

More than three decades after the discovery of high temperature superconductivity (SC) in cuprates, there is no consensus on the mechanism of the phenomenon. There is broad agreement that the undoped parent antiferromagnetic compounds can be described within the Cu-only one-band two-dimensional (2D) Hubbard model, which ignores the O-ions entirely. Proximity of SC to antiferromagnetism has led to the widely held belief that the mechanism of SC can also be found within an effective weakly-doped single-band Hubbard model [1–4] based on the claim that the spins on the Cu-sites form local spin-singlets that behave like double occupancies in the single-band Hubbard model [5]. The list of approximate correlated-electron theories that find SC within the weakly doped one-band Hubbard model is long, but accurate numerical studies have consistently found that superconducting correlations are suppressed by the Hubbard $U$ for carrier concentrations believed to be appropriate for the superconductors [6, 7]. Recent very careful study using two distinct and complementary numerical approaches to calculating superconducting pair-pair correlations has concluded that SC is absent in the square lattice Hubbard model proximate to $\frac{1}{4}$-filling [8]. Inclusion of second neighbor hopping $t'$ beyond nearest neighbor (n.n.) does not change this conclusion [9, 10]. Signatures of pair-correlations enhanced by the Hubbard $U$ have been found uniquely at $\frac{1}{4}$-filling [11], far from the carrier concentration believed to be appropriate for the cuprates. A recent density matrix renormalization group (DMRG) calculation has claimed transition from $p$-wave to $d$-wave SC within the hole-doped triangular lattice Hubbard model, but once again at fillings very far away from $\frac{1}{2}$ [12].

A key reason for the continued application of the one-band Hubbard model to cuprates is the repeated finding that the ground state of the weakly doped 2-leg one-band Hubbard ladder is a Luther-Emery liquid, with gapless charge and gapped spin modes [13–19]. Such a spin-gap proximity effect has been considered essential for SC within an entire class of theories [1, 3, 17, 20]. DMRG calculations, highly precise for one dimensional (1D) Hamiltonians, find slower than $1/r$ decay of the superconducting pair-pair correlation $P(r)$ in the doped 2-leg one-band Hubbard ladder, where $r$ is the interpair separation [14, 15, 18, 19]. Power law decay slower than $1/r$ is a requirement as well as signature of quasi-long range order in one dimension [21]. Strong superconducting correlations in the doped ladder is a consequence of spin-singlet formation on the undoped ladder rungs [22]. The DMRG results therefore have lent credence to the viewpoint that some variant of the 2D one-band Hubbard model with minor modifications might still yield

![FIG. 1. Cuprate ladder geometries considered by us. Filled (open) circles represent copper (oxygen) atoms. (a) Ladder with three oxygen atoms per rung. (b) Ladder with five oxygen atoms per rung.](arXiv:2010.10609v2 [cond-mat.str-el] 13 Sep 2021)
A realistic description of the cuprate ladder, however, should include the oxygen\( (O)\)-ions (see Fig. 1). Surprisingly, few authors have investigated the appropriateness of replacing the more complete three-band 2-leg ladder Hamiltonian that includes the \( O \)-ions with the one-band Hubbard Hamiltonian \( H_{\text{Hubbard}} \). We have performed accurate DMRG calculations on long three-band 2-leg ladders for parameters appropriate for real cuprates. In order to reach the longest ladders possible, we have performed the bulk of our calculations for the geometry of Fig. 1(a), with three \( O \)-ions per ladder rung. We have also performed limited calculations of superconducting pair correlations for a shorter ladder with the geometry of Fig. 1(b), with \( O \)-ions outside the ladder bonded to the \( Cu \) sites. We find that that the distance-dependence of the superconducting pair correlations are independent of geometry, and are strongly suppressed for both geometries of Fig. 1 at the doping traditionally assumed to correspond to the maximum of the superconducting dome within a one-band picture, \( \delta \approx 0.125 \). We further determine the Luther-Emery correlation exponent, \( \kappa_{\text{p}} \), in the thermodynamic limit through fits of the charge density, finding \( \kappa_{\text{p}} < 1 \) for \( \delta = 0.125 \), consistent with the suppression of pairing. We present physical arguments within an effective Hamiltonian that explain the suppression of the superconducting pair correlations and their rapid decay. These results have profound implications for any realistic modeling of cuprates.

II. THEORETICAL MODEL, PARAMETERS AND COMPUTATIONAL TECHNIQUES

The one-band ladder Hamiltonian has parameters \( U \), the Hubbard repulsion; and the leg and rung hopping integrals \( t \) and \( t_{\perp} \), respectively. It is customary to express \( U \) and \( |t_{\perp}| \) in units of \( |t| \). Here we consider the three-band ladder Hamiltonian,

\[
H = \Delta_{dp} \sum_{i,\sigma} p_{i,\sigma}^\dagger p_{i,\sigma} + \sum_{i,j,\lambda,\sigma} t_{dp}^{\perp,i,j} \left( d_{i,\lambda,\sigma}^\dagger p_{j,\sigma} + H.c. \right) + \sum_{i,j,\lambda,\sigma} t_{dp}^{i,j} \left( d_{i,\lambda,\sigma}^\dagger p_{j,\sigma} + H.c. \right) + \sum_{i,j,\lambda,\sigma} t_{pp}^{i,j} \left( p_{i,\sigma} p_{j,\sigma} + H.c. \right) + U_d \sum_{i,\lambda} \left( d_{i,\lambda,\uparrow} d_{i,\lambda,\downarrow} + U_p \sum_{j} p_{j,\uparrow} p_{j,\downarrow} \right)
\]

(1)

Here \( d_{i,\lambda,\sigma}^\dagger \) creates a hole with spin \( \sigma \) on the \( i \)th \( Cu \) \( d_{x^2-y^2} \) orbital on the \( \lambda \)-th leg \( (\lambda = 1, 2) \), \( p_{i,\sigma}^\dagger \) creates a hole on the n.n. rung oxygen \( O \) or leg oxygen \( O \lambda \); \( t_{dp}^{\perp,i,j} \) and \( t_{dp}^{i,j} \) are n.n. ladder rung and leg \( Cu-O \) hopping integrals and \( t_{pp}^{i,j} \) is the n.n. \( O-O \) hopping integral. For the lattice of Fig. 1(a), the \( Cu-O \) hopping matrix elements along the legs of the ladder have the sign convention \( t_{dp}^{i,j} = -t_{dp} \) for \( j = i + \delta/2 \) and \( t_{dp} \) for \( j = i + \delta/2 \). Along the rungs of the ladder \( t_{dp}^{\perp,i,j} = -t_{dp}^{\perp} \). Similarly \( t_{pp}^{i,j} = \pm t_{pp} \), with the plus and minus signs occurring for \( j = i + \delta/2 \pm \delta/2 \), respectively (see Fig. 2). For the lattice of Fig. 1(a) we choose the orbital parities so that the added \( O \)-ions with the one-band \( H_{\text{Hubbard}} \) are n.n. ladder rung and leg \( Cu-O \) hopping integrals and \( t_{pp}^{i,j} \) is the n.n. \( O-O \) hopping integral. For the lattice of Fig. 1(a), the \( O \)-ions are strongly suppressed for both geometries of Fig. 1 at the doping traditionally assumed to correspond to the maximum of the superconducting dome within a one-band picture, \( \delta \approx 0.125 \). We further determine the Luther-Emery correlation exponent, \( \kappa_{\text{p}} \), in the thermodynamic limit through fits of the charge density, finding \( \kappa_{\text{p}} < 1 \) for \( \delta = 0.125 \), consistent with the suppression of pairing. We present physical arguments within an effective Hamiltonian that explain the suppression of the superconducting pair correlations and their rapid decay. These results have profound implications for any realistic modeling of cuprates.

FIG. 2. (Color online) Orbital parity and sign convention for the hopping matrix elements for the ladder geometry of Fig. 1(a). Orbital parity and signs for the lattice of Fig. 1(b) follow a similar convention (see text).
TABLE I. Average extrapolated charge densities on Cu and O-sites in the undoped and doped (δ = 0.125) three-band Hamiltonian for $U_d = 8$.

| $U_p$ | $t_{pp}$ | $\langle n_{Cu} \rangle$ | $\langle n_{O_R} \rangle$ | $\langle n_{O_L} \rangle$ |
|-------|----------|----------------|----------------|----------------|
| 0     | 0.0      | 0.81          | 0.13            | 0.19           |
| 0     | 0.5      | 0.73          | 0.22            | 0.28           |
| 3     | 0.0      | 0.82          | 0.12            | 0.18           |
| 3     | 0.5      | 0.75          | 0.20            | 0.26           |

In what follows, the computational results are for the geometry of Fig. 1(a), unless it is explicitly mentioned that they are for the geometry of Fig. 1(b).

III. COMPUTATIONAL RESULTS

In what follows, the computational results are for the geometry of Fig. 1(a), unless it is explicitly mentioned that they are for the geometry of Fig. 1(b).

A. Charge densities

In Table I we have given the calculated $L \rightarrow \infty$ extrapolated charges (see Supplemental Material [28] for the details of the extrapolation procedure) on the Cu ions ($n_{Cu}$), rung O-ions ($n_{O_R}$) and leg O-ions ($n_{O_L}$), respectively, for $\delta = 0$ and $\delta = 0.125$, which are representative for other $\delta$ (see Supplemental Material [28]). The doping-induced increase in $\langle n_{Cu} \rangle$ is very small, with the bulk of the doped charge going to O-ions. Importantly, given that there occur two leg O-ions corresponding to each rung O, the overall increase in population due to doping is larger for O$_R$ than O$_L$. Our calculated chargedensities are close to those obtained previously for shorter three-band ladders for similar parameters [24]. The calculated Cu-ion charge densities are very close to those obtained previously for shorter one-band ladders, where also a maximum near doping is the spin gap in the undoped state, the more rapid is the suppression of the spin gap with doping. This is particularly obvious from comparison of $t_{dd}^+ = 1.25$ versus 1.0. Equally interesting is the strong enhancement of $\Delta_S$ in the undoped state when $t_{pp} \neq 0$, as noted above, but...
very rapid suppression of the same upon doping. We further note that the detrimental effects of nonzero \( U_p \) and \( t_{pp} \) are synergistic, as seen from the inset of Fig. [4(b)], where the spin gap at \( \delta = 0.0625 \) for \( (U_p, t_{pp}) = (3.0, 0.0) \) and \( (3.0, 0.5) \) are the same, even as for \( \delta = 0 \) the spin gap is larger by more than a factor of 2 for \( (U_p, t_{pp}) = (3.0, 0.5) \). The very large \( \Delta_S \) for \( \delta = 0 \), \( t_{dp} = 1.25 \), along with \( \Delta_S \cong 0 \) for the doped cases here are in agreement with previous one-band calculation of the spin gap in the doped ladder [30] for \( U = 8 \) and \( t_\perp/t > 1.5 \).

The very rapid diminishing of \( \Delta_S \) with doping already suggests the suppression of the superconducting correlations we find (see below).

C. Superconducting pair-pair correlations

1. Rung singlet pairs

For direct comparison of superconducting correlations with single-band ladders we have evaluated the pair-pair correlation function \( P(r) = \langle P_i^\dagger P_j \rangle \), with \( r = |i - j| \), where \( P_i^\dagger \) is the Cu-Cu ladder rung spin-singlet (see Fig. [4(a)]), defined as \( 2^{-1/2}(d_{i,1,\uparrow}d_{i,2,\downarrow} - d_{i,1,\downarrow}d_{i,2,\uparrow}) \). Figs. [5]a and (b) show the ladder length dependence of \( P(r) \) for two different parameters sets, Fig. [5]a) with \( U_p = t_{pp} = 0 \) and Fig. [5]b) with \( U_p = 3 \) and \( t_{pp} = 0.5 \). For all of the ladder lengths and parameter values we studied, \( P(r) \) was well fit by a power law \( r^{-\alpha} \), provided short and long distances are excluded. These limits are due to finite size effects and are well understood in the case of the one-band ladder [18]. In particular, the sharp decrease in \( P(r) \) for \( r > L/2 \) in Figs. [5] and [6] is a finite-size effect and not due to insufficiently large DMRG m.

As seen in Fig. [6]a), for \( U_p = t_{pp} = 0 \) we find \( \alpha \sim 1 \). With more realistic parameters, \( U_p = 3 \) and \( t_{pp} = 0.5 \), we find the power law exponent \( \alpha \) close to 1.5 (see Fig. [6]b)).

In Fig. [6] we show power-law fits for \( \delta = 0.0625 \) (Fig. [6]a) and \( \delta = 0.1250 \) (Fig. [6]b) for the 96-rung ladder. Nonzero \( U_p \) and \( t_{pp} \) both suppress \( P(r) \), and
FIG. 7. (Color online) Rung-singlet $P(r)$ for the 64-rung lattice with $U_d = 8$, $U_p = 3$, $t_{pp} = 0.5$, and $\delta = 0.0625$. $P(r)$ is normalized by its value at $r = 1$. Solid (open) symbols are for lattice of Fig. 1(a) (Fig. 1(b)). The solid (dashed) line are power laws $r^{-1}$ ($r^{-2}$).

when both are nonzero the suppression of $P(r)$ is further increased. This is consistent with the synergistic suppression of the spin gap in the doped ladder. As in the one-band ladder, we find that $\alpha$ increases rapidly with doping [18].

As mentioned above, we have also performed calculations of the rung singlet superconducting pair correlations for the ladder with the geometry of Fig. 1(b). The results of these calculations are shown in Fig. 7, where we compare the distance dependences of the normalized rung singlet pair-pair correlations for the two geometries of Fig. 1. The distance dependence of the pair correlations for the geometry of Fig. 1(b) with outer O ions included is as rapid as that for geometry of Fig. 1(a). As we point out below, this result is to be anticipated from physical reasonings.

2. Other pairing symmetries

Given that the doped holes primarily occupy the $O_R$ and $O_L$ sites investigation of pair-pair correlations beyond those involving simple rung singlets is important (note that the overall charges continue to reside primarily on the Cu-ions though). We investigated several different pair symmetries composed of superpositions of singlets on Cu and O atoms. The pair symmetries we investigated are shown in Fig. 8. We have calculated $P(r) = |i-j| \neq 1$ for these different pairing symmetries for a 32-rung ladder with $U_d = 8$, $\Delta_d = 3$, $U_p = 3$ and $t_{pp} = 0.5$, for doping $\delta = 0.125$. All $P(r)$ are normalized by their $r = 1$ value; we have taken absolute values of correlations that are negative.

![FIG. 8. (Color online) Pair-pair correlations for 32-rung ladders of Fig. 1(a) for the oxygen based pair symmetries in Fig. 4. Parameters are $U_d = 8$, $U_p = 3$, $t_{pp} = 0.5$, and $\delta = 0.125$. (a) pair symmetry of Fig. 4(b); (a) pair symmetry of Fig. 4(c); (c) pair symmetry of Fig. 4(d); (d) pair symmetry of Fig. 4(e); Round symbols are for Cu rung pairs (Fig. 4(a)), square open (filled) symbols are for $s$ and $d$-wave pairing of the specified type (see text).]

self, or in case of Fig. 4(b) a singlet between O atoms immediately adjacent to the Cu rung atoms.

2. $P(r)$ decays much faster with distance than the rung singlet correlation. This includes Figs. 4(c) and 4(d), Fig. 4(e) (d-wave only), Fig. 4(f) (d-wave only) and Fig. 4(g).

Based on these results we conclude that superconducting pair-pair correlations in the three-band ladder in general decay much faster than in the single-band ladder, and for realistic correlation and hopping parameters this decay precludes quasi-long range order.
D. Density oscillations

In the Luther-Emery phase, the long-distance decay of pair-pair correlations follows a power law determined by the correlation parameter \( \kappa_n \), with \( P(r) \propto r^{-1/\kappa_n} \) (\( \alpha = 1/\kappa_n \)). Similarly, density-density correlations \( N(r) \) follow a power law with \( N(r) \propto r^{-\kappa_n} \) \( (N(r = |i-j|) = \langle n_in_j \rangle - \langle n_i \rangle \langle n_j \rangle) \), where \( n_i \) is the charge density operator for site \( i \). Pairing correlations decay slower than \( 1/r \) and dominate over density-density correlations only for \( \kappa_n > 1 \). Density correlations provide a second estimate of \( \kappa_n \) and consistency check.

In the 2-leg one-band ladder, charge density (Friedel) oscillations can be fit to accurately extract \( \kappa_n \) \cite{18}. We use a similar procedure in our three-band model calculations. We fit the charge density to the following function \cite{18, 31}:

\[
\rho_i = n_i - \rho_i^{\text{background}} = A \frac{\cos(\pi n_i / L_{\text{eff}} + \phi)}{\sin(\pi j / L_{\text{eff}}^{\kappa_n/2})} + n_\text{total}.
\]

In Eq. \( \ref{eq:oscillation} \) \( n_i \) is the charge density in the \( j \)-th unit cell of the lattice; \( n_i \) is the sum of the charge densities of the rung copper and oxygen atoms, plus the charge densities on two adjacent leg oxygen atoms. \( N_h \) is the number of holes, \( A \) the overall amplitude, \( \phi \) a phase shift, and \( n_\text{total} \) the background charge density. \( L_{\text{eff}} \) is an effective length that is less than \( L \) because of the finite extent of holes \cite{18}. We performed a nonlinear fit of the charge density to Eq. \( \ref{eq:oscillation} \) in the central region of the ladders for \( L = 32, 48, 64 \), and \( 96 \), keeping \( A, n_\text{total}, \kappa_n \), and \( \phi \) as free parameters. Fig. \( \ref{fig:oscillation} \text{(a)} \) and \( \text{(b)} \) show representative fits for \( L = 96 \). While in the one-band ladder a good fit was found \cite{18} with \( L_{\text{eff}} = L - 2 \), we found a shorter \( L_{\text{eff}} \) in the three-band ladder, for example \( L_{\text{eff}} \approx L - 9 \) and \( L - 6 \) for \( \delta = 0.0625 \) and \( \delta = 0.125 \), respectively. This shows that doped holes extend over a larger number of lattice sites in the three-band ladder than in the one-band ladder (see also Section \( \ref{sec:oscillation} \)).

The value of \( \kappa_n \) can be most accurately determined in ladders \cite{18} from the scaling of the amplitude of the density oscillations in the center of the ladder,

\[
\delta n(L) = n(L/2) - n_0 \propto L^{-\kappa_n/2}.
\]

In Eq. \( \ref{eq:oscillation} \) we determined \( n(L/2) \) and \( n_0 \) from the fit of
Table II. Correlation exponents $\kappa_p$ obtained from fitting $P(r)$ (Section III C) and density oscillations (Section III D).

| $\delta$  | $U_p$ | $t_{pp}$ | $P(r)$ ($L=96$) | $\kappa_p$ | $\delta n$ ($L \to \infty$) |
|-----------|-------|----------|-----------------|------------|-----------------------------|
| 0.0625    | 0.0   | 0.0      | 1.14(4)         | 1.35(6)    |                             |
| 0.0       | 0.5   | 0.99(3)  | 1.22(2)         |            |                             |
| 3.0       | 0.0   | 1.01(3)  | 1.20(6)         |            |                             |
| 3.0       | 0.5   | 0.76(2)  | 0.97(1)         |            |                             |
| 4.0       | 0.6   | 0.65(2)  | 0.93(5)         |            |                             |
| 0.125     | 0.0   | 0.91(2)  | 1.08(6)         |            |                             |
| 0.0       | 0.5   | 0.78(2)  | 0.93(2)         |            |                             |
| 3.0       | 0.0   | 0.83(2)  | 1.08(3)         |            |                             |
| 3.0       | 0.5   | 0.65(2)  | 0.80(4)         |            |                             |
| 4.0       | 0.6   | 0.56(2)  | 0.75(8)         |            |                             |

Eq. 2 Fig. 11(c) shows typical results for $\delta n$ for two different parameter sets (see 28 for other parameter values). We then estimated $\kappa_p$ in the $L \to \infty$ limit from a linear fit as was done for the one-band ladder 18. Table II summarizes our results for $\kappa_p$ as determined from directly fitting $P(r)$ and from Eq. 3. In comparison, the value of $\kappa_p$ in the single band ladder is 1.54–1.66 at $\delta = 0.0625$ and 0.92–1.17 at $\delta = 0.125$ 18, roughly consistent with our $U_p = t_{pp} = 0$ values. In general, the $L \to \infty \kappa_p$ determined from density oscillations is larger than the value found from the $L = 96$ pair-correlations, with a larger finite-size correction at $\delta = 0.0625$ than at $\delta = 0.125$. A slight decrease in the power-law slope of $P(r)$ with increasing size is evident in Fig. 5 so we believe that the results from fitting $P(r)$ and $\delta n$ are consistent with each other.

We note that the $\kappa_p$ calculated from the two different methods display nearly identical dependence on $U_p$ and $t_{pp}$. The effects of nonzero $U_p$ and $t_{pp}$ are not simply additive. Rather (see Table II), the decrease of $\kappa_p$ is larger when both $U_p$ and $t_{pp}$ are nonzero compared to the sum of the changes in $\kappa_p$ with $(U_p > 0, t_{pp} = 0)$ or $(U_p = 0, t_{pp} > 0)$. We note that we cannot rule out the possibility that $\kappa_p > 1$ in the limit of very small doping; indeed we find $\kappa_p \sim 1$ for $\delta = 0.0625$ even with realistic $U_p$ and $t_{pp}$. However, if one takes the doping typically assumed as maximizing pairing in the 2D one-band Hubbard model ($\delta = 0.125$), we find that $\kappa_p$ is significantly less than one, even considering our computational and finite-size errors. This indicates the absence of the quasi-long range SC characteristic of the single-band ladder.

E. Suppression of pair correlations, a physical picture

The suppression of the pair-pair correlations within the multi-band model is reminiscent of similar suppression of the same correlations for large rung hopping $t_\perp > t$ within the one-band model (see Fig. 6 in reference 15). As seen in reference 12 not only is the one-band pair-pair correlation suppressed by large $t_\perp$, the suppression occurs at smaller and smaller $t_\perp$ (that are however $> 1$) as the Hubbard repulsion $U$ increases. Within the same range of $U$ the spin gap in the undoped one-band ladder increases with $U$. It therefore follows that increase in the spin gap in the undoped one-band ladder is accompanied by concomitant increase of pair correlations in the doped ladder, only until a maximum in the undoped ladder spin gap is reached. Beyond this maximum, further increase of the spin gap in the undoped single-band ladder results in suppression of the pair-pair correlations in the doped ladder. Our results in Figs 6 indicate that this maximum in the spin gap of the undoped three-band ladder has been reached already at $t_{pp}^\dagger = 1$. We argue in the following that this is due to the large pair-breaking effect in the multi-band ladder.

Superconducting pairing involving rung singlets in both one- and multi-band ladder Hamiltonians can understood within an effective Hamiltonian of the form,

$$H_{\text{eff}} = \sum_i J(\delta) P_i^\dagger P_i - t_{\text{pair}} \sum_{(i,j)} P_i^\dagger P_j - t_{f} \sum_{(\mu,\nu),\sigma} f_{\mu,\sigma}^\dagger f_{\nu,\sigma}$$

(4)

where $J(\delta)$ is proportional to the self-consistent spin gap at doping $\delta$, $t_{\text{pair}}$ the effective pair hopping integral, and $t_{f}$ refers to single-particle fermion hops. Here $i$ and $j$ refer to rung indices. While $\mu,\nu$ refer to Cu-ions on nearest neighbor rungs in the one-band ladder, they refer to both Cu- and O-sites in the multi-band ladder. Within the one-band model, $t_{\text{pair}}$ and $t_{f}$ are related, with $t_{\text{pair}} \sim t_\perp^2/\Delta_{pb}$, where $\Delta_{pb}$ is the pair-binding energy, roughly proportional to the spin gap in the doped ladder.

The interactions $J(\delta)$ and $t_{\text{pair}}$, taken together, dominate over the pair-breaking single-particle $t_f$ over a broad range of parameters in the one-band ladder, including in particular $t_{\perp} = 1$. This situation is altered significantly within the multi-band model. The doped holes now enter primarily O-sites (see Table 1), and the complete spin-singlet wavefunction involves not only the Cu-ions but also the rung O-ion and the four ladder oxygens on either side of the rung. Pair motion now must involve not only the doped charges on the Cu-ions of a rung, but also those on the neighboring O-ions, making the effective mass of the spin-singlet within the three-band model considerably larger than in the one-band model. At the same time, however, $t_\perp$ now can involve the holes on the O-ions exclusively, with the Cu-ion holes playing a very limited role (i.e., $t_\perp$ now includes and is even dominated by $t_{pp}$). Consequently, the effective $t_{\text{pair}}$ is smaller and the effective $t_{f}$ larger within the three-band model. Single-particle hopping thus has a far stronger pair-breaking effect in the three-band ladder.

Based on the above it now becomes obvious why the strongest suppression of the doped-state spin gap and rung singlet superconducting pair correlations occur within the Hamiltonians with nonzero $t_{pp}$ (see Figs. 3(b)}
and \( \mathbf{6} \). With the geometry of Fig. \( \mathbf{1} \)(b), the effective mass of the spin-singlet is further enhanced while the additional \( t_{pp} \) contribute to additional \( t_2 \) and pair-breaking. The strong suppression of pair correlations should therefore be common to the geometries of Fig. \( \mathbf{1} \)(a) and (b), as indeed is found numerically.

IV. DISCUSSIONS AND CONCLUSION

Our theoretical results demonstrate that, (i) conclusions regarding pairing based on effective single-band ladder models cannot be extended to the three-band ladder, and (ii) there is no pairing within the three-band ladder for realistic cuprate parameters \( U_p = 3-4, t_{pp} = 0.5-0.6 \) [2]. \( U_p \) and \( t_{pp} \) both suppress pairing uniformly.

The absence of SC in the 2-leg ladder compound \( \text{La}_{2-y}\text{Sr}_y\text{CuO}_2 \), \( y = 0.12 \) is therefore expected within our theory. Superconducting \( \text{Sr}_{14-4x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41} \) consists of alternating planes of corner-sharing \( \text{CuO}_2 \) chains and edge-sharing \( \text{CuO}_3 \) ladders [32, 33]. It is believed that there occur nearly 5 holes per formula unit (f. u.) on chains and 1 hole per f. u. on ladders at \( x = 0 \). There occurs some transfer of holes from chain to ladder with increasing \( x \), but the actual extent of the transfer is not agreed upon [30]. The appearance of SC above 4.0 GPa in \( x = 11.5 \) single crystals is accompanied by a 1D-to-2D dimensional crossover, as evidenced from the insulator-like resistivity \( \rho_a \) along the rung-axis \( a \) at all temperatures below the critical pressure and metallic \( \rho_a \) at all temperatures above this pressure [34]. The resistivity ratio \( \rho_a/\rho_c \) (the \( c \)-axis corresponds to the ladder leg direction) of the \( x = 11.5 \) compound decreases by more than a factor of 4 at low temperature and high pressure [34]. There occurs a concomitant decrease in the \( a \)-axis lattice parameter, although at still higher pressure where superconducting \( T_c \) decreases the lattice parameter increases again. \( ^{63}\text{Cu} \) and \( ^{17}\text{O} \) NMR studies for the \( x = 12 \) compound have found that the spin gap decreases sharply with pressure, and there appear low-lying spin excitations, indicating the presence of mobile quasi-particles that contribute to a finite density of states at the Fermi level and perhaps also SC [37, 38]. Taken together, these observations, (i) indicate clearly that the origin of SC in \( \text{Sr}_{14-4x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41} \) cannot be found within ladder-based theories [33], and (ii) are consistent with our finding that superconducting correlations are absent in the three-band ladder Hamiltonian with realistic \( U_p \) and \( t_{pp} \).

Our results raise a fundamental (and disturbing) question. What is the implication of the absence of a Luther-Emery superconducting phase \( \mathbf{12} \) in the three-band 2-leg ladder Hubbard Hamiltonian for the 2D \( \text{CuO}_2 \) layer? We make the following observations. First, theories of cuprate SC that assume a gapped spin-liquid phase proximate to the superconducting state [3, 17, 20, 39] cannot be justified by the demonstration of quasi-long range superconducting correlations within the one-band ladder-based theories. The one-band ladder model is an artificial one with no relationship to real cuprates. Second, the profound difference between the results of one- and three-band ladder calculations (understandable physically with hindsight, see Section III.D) suggests that the mapping of the three-band Hamiltonian to the one-band Hubbard model \( \mathbf{5} \) is correct only for a limited choice of parameters. In the context of cuprates, the applicability of the mapping across doping levels, realistic geometries and parameters (especially \( t_{pp} \)) has been questioned by other authors [40, 44], although these criticisms themselves remain controversial. Our work suggests that re-evaluation of these earlier works is necessary. Finally, as with the 2D one-band Hubbard Hamiltonian, numerical computation of \( d_{x^2-y^2} \) pair correlations within the three-band Hamiltonian for the \( \text{CuO}_2 \) layer also found absence of SC [43]. This latter work used the constrained path quantum Monte Carlo approach that relies on a trial wavefunction to eliminate the Fermion sign problem. The calculations were also based on relatively small lattices. Our DMRG calculations, devoid of sign errors, provide strong support to the conclusions of reference 43. Taken together, these observations suggest that a comprehensive theory of cuprate SC may require starting hypotheses or models that are significantly different from existing ones.

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