

Towards effective models for low-dimensional cuprates: From ground-state Hamiltonian reconstruction to spectral functions

Hannah Lange ^{1,2,3} Tizian Blatz ^{1,3} Ulrich Schollwöck ^{1,3} Sebastian Paeckel ^{1,3} and Annabelle Bohrdt ^{1,3}

¹*Department of Physics and Arnold Sommerfeld Center for Theoretical Physics (ASC),*

Ludwig-Maximilians-Universität München, Theresienstrasse 37, München D-80333, Germany

²*Max-Planck-Institute for Quantum Optics, Hans-Kopfermann-Strasse 1, Garching D-85748, Germany*

³*Munich Center for Quantum Science and Technology, Schellingstrasse 4, Munich D-80799, Germany*



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Understanding which minimal effective model captures the essential physics of cuprates is a key step towards unraveling the mechanism behind high- T_c superconductivity. Recent measurements of the dynamical spin structure factor (DSF) in cuprate ladder compounds have indicated the presence of an additional, attractive term in the single-band Hubbard model, potentially originating from electron-phonon interactions. Here, we demonstrate that similar DSF features can also be captured by t - J descriptions with a smaller attractive term. Motivated by this observation, we systematically investigate the strength and origin of different contributions to the single-band Hamiltonians by downfolding either from the three-band Emery model or the electron-phonon coupled Hubbard-Holstein model. For one-dimensional systems, we find that the extended versions of both single-band descriptions can reproduce the experimentally observed DSF signatures. Finally, we extend our analysis to two dimensions by comparing two-hole correlation functions for the different single-band models. Our results provide new insights into the long-standing question of which single-band Hamiltonian can capture the essential physics of cuprates.

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The discovery of superconductivity in LaBaCuO [1] has inspired decades of extensive experimental and theoretical research into cuprate materials. The common belief is that the relevant physics takes place in the copper oxide planes, with each CuO₂ unit cell consisting of a copper $d_{x^2-y^2}$ orbital and two oxygen $p_{x,y}$ orbitals, which is described by the three-band Emery model [2]. However, this model is very challenging to simulate for most methods—although methods like dynamical mean-field theory [3,4] allow for multiband simulations under the assumption of local interactions and correlations [5]—and hence they are often downfolded to a single-band description. However, which single-band model can most accurately capture the cuprate physics, how large the corresponding Hamiltonian parameters are, which terms are required, and which terms can be neglected have remained unclear until today. After decades of study, this question has recently regained attention, as large-scale numerical simulations suggest that additional Hamiltonian terms might be essential for capturing the cuprate physics [6,7]. Furthermore, increasing experimental evidence also points toward the need for more complex models beyond the standard Hubbard model [8–10]. Thus, novel downfolding procedures yielding effective lattice models with potentially long-ranged

interactions, can provide new insights into the relevant physics of real materials [6].

In the earliest works, downfolding was typically done by constructing a new basis set of wave functions that are centered at the copper sites. In a perturbative analysis, Zhang and Rice argued that upon doping with a single hole, this new basis consists of additional holes delocalized over the p -sites, forming singlets with the neighboring d -hole [11]. These so-called *Zhang-Rice singlets* have also been observed, both experimentally and numerically; see, e.g., Refs. [12–16]. In the limit of small hopping integrals between the orbitals, one arrives at the single-band t - J model,

$$\hat{\mathcal{H}}_{t,J} = \hat{\mathcal{P}}_G [\hat{\mathcal{H}}_t + \hat{\mathcal{H}}_{3s}] \hat{\mathcal{P}}_G + J \sum_{\langle i,j \rangle} \left(\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - \frac{1}{4} \hat{n}_i \hat{n}_j \right), \quad (1)$$

with the Gutzwiller projector $\hat{\mathcal{P}}_G$ projecting on singly occupied sites, and the kinetic terms $\hat{\mathcal{H}}_t = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.})$ and $\hat{\mathcal{H}}_{3s} = -t_3 \sum_{\langle i,j,k \rangle, \sigma} (\hat{c}_{k\sigma}^\dagger \hat{n}_{j\bar{\sigma}} \hat{c}_{i\sigma} - \hat{c}_{k\sigma}^\dagger \hat{c}_{j\bar{\sigma}}^\dagger \hat{c}_{j\sigma} \hat{c}_{i\bar{\sigma}} + \text{H.c.})$. We denote indices corresponding to neighboring lattice sites by $\langle \cdot, \cdot \rangle$. Similar results have been obtained e.g., in Refs. [17–22]. In some of the works, additional terms like density-density interactions, further-range, or density-assisted hopping terms are introduced [6,7].

When allowing for larger occupations, an effective single-band Fermi-Hubbard model can be derived [6,17,21,22],

$$\hat{\mathcal{H}}_{\text{FH}} = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}. \quad (2)$$

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Intriguingly, recent comparisons of resonant inelastic x-ray scattering (RIXS) and angle-resolved photoemission spectroscopy (ARPES) on one-dimensional (1D) cuprates with numerics for the single-band Hubbard model have shown that attractive interactions ($V_d < 0$) for neighbors with distance d of the form

$$\hat{\mathcal{H}}_V = \sum_{\langle i,j \rangle_d} V_d \hat{n}_i \hat{n}_j \quad (3)$$

need to be included to account for the observed features of the dynamical structure factor (DSF) and the photoemission spectrum, mostly limited to nearest-neighbor $V := V_{d=1}$ terms on the order of $V \approx -t$. In this work, $V' := V_{d=2}$ will also be considered. This attraction could potentially be induced by electron-phonon interactions [10,22–27]. For ladder compounds, RIXS and neutron scattering measurements have recently demonstrated the necessity to include similar attractive interactions [8,9].

In this work, we systematically analyze the Fermi-Hubbard model and compare it to the t - J model, both with and without additional terms beyond the standard versions such as attraction or density-assisted hopping. We begin by investigating 1D and ladder compounds, focusing on the origin of the potential attractive interactions and their impact on the spectral properties. Then, we extend our analysis to the 2D case. Specifically, we (i) compare the DSF for ladder compounds within the t - J and Fermi-Hubbard models with and without nearest-neighbor attraction, finding that both reproduce spectral features consistent with resonant RIXS measurements; (ii) explore the microscopic origin of the attractive interaction as well as other additional terms by applying ground-state reconstruction schemes based on the Hubbard-Holstein model with electron-phonon coupling and three-band Fermi-Hubbard models; (iii) validate the reconstructed models by computing the DSF, which again shows good agreement for both the FH + V and t - J models; and (iv) extend the analysis to two dimensions by comparing correlation functions for the different effective one-band models.

Our work is relevant from both methodological and physical perspectives. From a methodological standpoint, our contribution lies in the development of reduction schemes to derive single-band models starting from either the electron-phonon coupled Hubbard-Holstein model or the three-band Emery model, which are based on a novel application and combination of algorithms from Refs. [6,28]. Specifically, we extend the Hamiltonian reconstruction scheme of Ref. [28], originally developed to reconstruct spin Hamiltonians from measurements of the same system, to the Hubbard-Holstein model and apply it in a downfolding context to obtain effective descriptions such as the single-band Fermi-Hubbard and t - J models. Moreover, by combining this approach with the framework of Ref. [6], we enable reconstructions of the three-band model to not only the single-band Fermi-Hubbard but also t - J Hamiltonians. From a physical perspective, our study provides new insights into cuprate compounds in three key aspects: (i) a unified analysis across different dimensionalities, ranging from one-dimensional chains to ladders and two-dimensional systems; (ii) a systematic comparison between the t - J model originally derived by Zhang and Rice [11] and Fermi-Hubbard-based reconstructions; and (iii) a direct

comparison between downfolding results obtained from the Emery and Hubbard-Holstein models.

I. RESULTS

A. Ladder compounds

As a general motivation for our work, we consider the recent experiments probing the dynamical spin structure factor (DSF) of the cuprate ladder compounds on $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ [8] and $\text{Sr}_{2.5}\text{Ca}_{11.5}\text{Cu}_{24}\text{O}_{41}$ [9] at hole doping $\delta = 6\%$. The magnetic excitations of these systems are theoretically well understood: in an isotropic, undoped ladder, the ground-state consists of spin singlets on the rungs, and the elementary magnetic excitations are triplets, leading to a continuum of two-triplon excitations [29]. Upon doping, holes break spin singlets and give rise to quasiparticles with loosely bound spin and charge components, which in turn contribute spin-flip excitations to the DSF. In Fig. 1(a), we show the RIXS measurement from Ref. [8] at 260 K (left panel) at hole doping $\delta = 6\%$, where the two-triplon continuum is clearly visible, while spin-flip excitations are strongly suppressed. This behavior is in stark contrast to results from a bare Fermi-Hubbard ladder of length $L_x = 33$ [see Fig. 1(a), second panel], obtained via density matrix renormalization group [DMRG, see the Supplemental Material (SM) [30] and Refs. [31–35] therein]) using hopping parameters $t_{\perp}/t = 0.84$ and $t_{\text{diag}}/t = -0.3$ as extracted in Ref. [8]. In the Fermi-Hubbard case, prominent spin-flip excitations with downward dispersion near the Brillouin zone boundary appear below the two-triplon continuum—features that are absent in the experiment. Notably, the three-band Hubbard model has also been shown to not capture this suppression [16]. To reconcile theory and experiment, Refs. [8,9] proposed the inclusion of a nearest-neighbor attraction of strength $V/t = -1.25$ along both ladder directions and a rescaled on-site interaction $U/t = 8 + V$. The attraction V increases the rung-pairing correlations significantly [8,36], and the stronger pairing suppresses the spin-flip contributions [Fig. 1(a), third panel]. However, the bare t - J model—without any additional attraction—naturally features strong pairing for holes in different legs of the ladder [37,38]. As we show here, this intrinsic pairing of the bare t - J ladder gives rise to a similar pairing strength as for the FH + V ladder, and consequently to very similar features in the DSF: spin-flip excitations are suppressed, and the energy of the spectral peak at the Brillouin zone boundary $k = \pi$ aligns closely with that observed in experiment [see Fig. 1(a), fourth panel and Fig. 1(b)].

In general, the spectral weight is shifted towards $\pi/2$ for the RIXS, which is not the case for the inelastic neutron scattering results in Ref. [9]. More information on the theoretical DSF can be found in the SM [30].

The similar pairing strength for both FH + V and t - J models can be quantified in terms of the binding energies $E_B = 2E(N^h - 1) - E(N^h) - E(N^h - 2)$ (where $N^h = \delta L_x L_y$ is the number of holes): For $L_x = 64$, the FH + V ladder (with $t_{\text{diag}} = 0$) features binding energies $E_B^{\text{FH}+V}/t = 0.23$, which is comparable to those of the bare t - J ladder (with $J_{\parallel}/t = 0.5$, $J_{\perp}/t = 0.35$, $J_{\text{diag}} = t_{\text{diag}} = 0$), $E_B^J/t = 0.17$. Both are much larger than $E_B^{\text{FH}}/t = 0.09$ for the bare Fermi-Hubbard ladder.

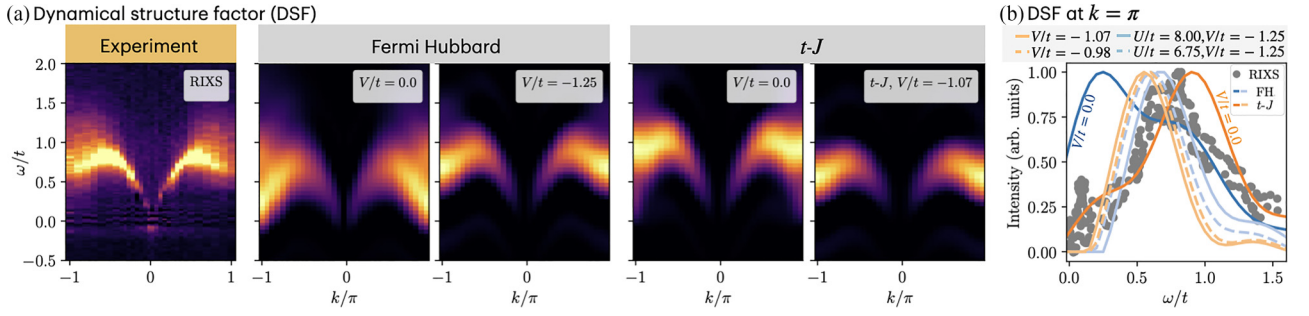


FIG. 1. The effective model for cuprate ladders. (a) We compare the dynamical structure factor (DSF) obtained from RIXS measurements on $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ [8] (left) to four different effective model candidates: The Fermi-Hubbard model without and with attractive interactions $V/t = -1.25$ and rescaled $U/t = 8 + V$ (FH and FH + V), the bare t - J model without attraction, and the t - J model with attraction $V/t = -1.07$ (t - J + V) for ladders of length $L = 33$ and $\delta = 6\%$ hole doping (left to right). (b) FH + V (light blue), bare t - J (dark orange), and t - J + V (light orange) models agree well with recent RIXS measurements [8], as shown for exemplary momentum $k = \pi$. Dashed lines refer to FH + V and reconstructed t - J + V without rescaled on-site interaction $U/t = 8$.

To enable a more systematic comparison between the different single-band models, we employ a reconstruction scheme to derive an effective t - J Hamiltonian that reproduces the ground-state of the FH + V ladder with and without rescaled U ; see the SM. We find that the interaction term V is suppressed to $V/t = -1.07$ and -0.98 , respectively. In both cases, the resulting DSF closely resembles the DSF for the FH + V model; see Fig. 1(a) (right).

These observations show that both the Fermi-Hubbard model with attraction (FH + V) and the considered t - J models with and without attraction appear to be suitable effective single-band models for the cuprate ladder compounds. Due to their close connection to two-dimensional compounds, this raises a more fundamental question: What range, strength, and sign of interactions should be included in an effective model to faithfully capture the essential physics of cuprate materials?

B. One-dimensional compounds

In the following, we address this question by employing ground-state reconstruction schemes to determine the best effective single-band description from the three-band and Hubbard-Holstein models, and comparing their spectral features to RIXS results from the 1D cuprate compound $\text{Ba}_2\text{CuO}_{2+\delta}$ [10]. More precisely, for the three-band model, we consider the hole-doped three-band model,

$$\hat{\mathcal{H}}_{3b} = -t_{pd} \sum_{\langle ij \rangle \sigma} (\hat{a}_{i\sigma}^\dagger \hat{p}_{j\sigma} + \text{H.c.}) - t_{pp} \sum_{\langle\langle ij \rangle\rangle \sigma} (\hat{p}_{i\sigma}^\dagger \hat{p}_{j\sigma} + \text{H.c.}) + \sum_{\mu \in \{p,d\}} U_\mu \sum_i \hat{n}_{i\uparrow}^\mu \hat{n}_{i\downarrow}^\mu + \Delta_{pd} \sum_{i\sigma} \hat{p}_{i\sigma}^\dagger \hat{p}_{i\sigma}, \quad (4)$$

with orbital-dependent on-site interactions $U_{d,p} > 0$ and hoppings $t_{pd,dd}$, as well as a potential offset of the oxygen orbitals $0 < \Delta_{pd} < U_d$. The annihilation (creation) operators $\hat{d}^{(\dagger)}$ and $\hat{p}^{(\dagger)}$ create holes on copper and oxygen sites, respectively. The half-filled case ($n = 1$) is defined by one hole per unit cell.

For the Hubbard-Holstein model, we include electron-phonon interactions given by the extended Hubbard-Holstein

Hamiltonian

$$\hat{\mathcal{H}}_{\text{HH}} = \hat{\mathcal{H}}_{\text{FH}} + \omega_0 \sum_i \hat{b}_i^\dagger \hat{b}_i + g_0 \sum_i \hat{n}_i (\hat{b}_i^\dagger + \hat{b}_i) + g_1 \sum_{\langle i,j \rangle} \hat{n}_i (\hat{b}_j^\dagger + \hat{b}_j), \quad (5)$$

with phonon operators $\hat{b}^{(\dagger)}$, phonon frequency ω_0 , and on-site (nearest-neighbor) electron-phonon coupling $g_{0(1)}$. The strength of the resulting effective attraction, and its impact on spectral features, has been considered, e.g., in Refs. [10,23,25,27], suggesting an effective attraction on the order of $-t$, similar to that found in ladder compounds. Note that despite the effective attraction that can be derived from this model, it cannot explain the emergence of unconventional superconductivity due to the large effective mass of the bipolaronic two-electron bound states [39].

The reconstruction we perform proceeds as follows: Starting from ground-states of (i) the Hubbard-Holstein model (5) with $\omega_0/t = 0.2$, $g_0/t = 0.3$, $g_1/t = 0.15$ (as estimated in Ref. [27]) and (ii) the three-band Emery model (4) with $t_{pp}/t_{pd} = 0.5$, $U_d/t_{pd} = 6.0$, $U_p/t_{pd} = 3.0$, $\Delta_{pd}/t_{pd} = 3.5$ as used in Ref. [6], we construct the effective FH + V and t - J (+ V) Hamiltonians; see Fig. 2. For the reconstruction from (i), this amounts to finding the effective model for which

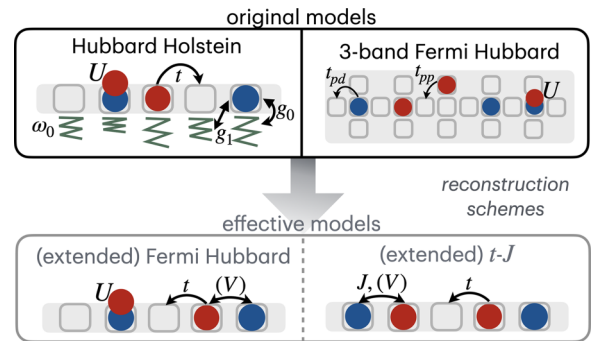


FIG. 2. Ground-state reconstruction schemes: We start from Hubbard-Holstein or three-band Fermi-Hubbard chains (top) and reconstruct the corresponding effective single-band Fermi-Hubbard or t - J models (bottom).

the energy variance measured with respect to the original ground-state is minimal [28]. This condition can be rewritten in terms of a correlation matrix, with the eigenvalues corresponding to the variance of an effective Hamiltonian given by the corresponding eigenvector. While the algorithm was initially developed for reconstructing spin Hamiltonians from measurements of the same system, here we extend its use to the Hubbard-Holstein model and apply it as a downfolding method. In analogy to a Lang-Firsov transformation of the Hubbard-Holstein Hamiltonian, where additionally a next-nearest-neighbor interaction V' arises, we also include this term in this case. For (ii), we construct the Wannier functions centered at the copper site in order to construct a unitary transformation from the three-band to the single-band description [6] and apply the reconstruction scheme from (i) afterwards. In the following, we briefly outline the two downfolding schemes. Further details can be found in the SM [30].

1. Downfolding from the Hubbard-Holstein model

The downfolding approach described here is built on the Hamiltonian reconstruction scheme from Ref. [28]. The goal of the reconstruction is to find the operator $\hat{\mathcal{H}}_{\text{eff}}$ for which the variance with respect to the ground-state of the original Hamiltonian, v , is reduced. Formally, we minimize

$$\langle \hat{\mathcal{H}}_{\text{eff}}^2 \rangle_v - \langle \hat{\mathcal{H}}_{\text{eff}} \rangle_v^2 = \epsilon, \quad (6)$$

where $\langle \cdot \rangle_v$ denotes the expectation value in the state v , and $\epsilon \in \mathbb{R}$. To do that, we construct $\hat{\mathcal{H}}_{\text{eff}}$ from a set of $\{L_i\}$ that span the space of the effective Hamiltonian, i.e., $\hat{\mathcal{H}}_{\text{eff}} = \sum_i w_i \hat{L}_i$. More precisely, we use the translationally invariant formulation of this scheme, in which we denote the Fourier-transformed operator basis as $\{\tilde{L}_{q\alpha}\}$, where q is the momentum and

$$\tilde{L}_{q\alpha} = \frac{1}{\sqrt{n}} \sum_{x=1}^n L_{x\alpha} e^{iqx}. \quad (7)$$

The key object in this reconstruction is then given by the (translationally invariant) correlation matrix:

$$\tilde{M}_{p\alpha, q\beta}^{(v)} = \frac{1}{2} \langle \{\tilde{L}_{p\alpha}, \tilde{L}_{q\beta}\} \rangle_v - \langle \tilde{L}_{q\alpha} \rangle_v \langle \tilde{L}_{p\beta} \rangle_v. \quad (8)$$

In this formulation, only the zero-momentum sector of the correlation spectrum is relevant for reconstructing a translationally invariant Hamiltonian from its eigenstate. The condition (6) above can then be reformulated as an eigenvalue problem, $w^T M^{(v)} w = \epsilon$ [28].

An effective Hamiltonian can be reconstructed if the eigenvalue spectrum of $M^{(v)}$,

$$\text{spec}(M^{(v)}) = \{\lambda_i^{(v)}\}_{i=1}^N, \quad (9)$$

with $\lambda_i^{(v)}$ ordered from the lowest to the highest eigenvalue, satisfies $\lambda_2^{(v)} > 0$ [28]. Specifically, if $\lambda_1^{(v)} = 0$, then the effective Hamiltonian is uniquely determined. The corresponding eigenvector encodes the reconstructed Hamiltonian parameters. In our setting, where the reconstruction is performed in a different Hilbert space than the original, exact recovery is not possible, and we find that all $\lambda_2^{(v)} > 0$. In this case, the smallest eigenvalue $\lambda_1^{(v)}$ serves as a measure of the reconstruction error.

TABLE I. Reconstructed parameters for ground-state Hamiltonian reconstruction of Hubbard-Holstein (HH) and three-band Fermi-Hubbard (FH) chains to effective single-band Fermi-Hubbard and t - J models without and with a nearest-neighbor density interaction Eq. (3) (top vs bottom). We omit the next-nearest-neighbor interaction V' for the t - J reconstruction here, since it is one order of magnitude smaller than for FH; see the SM [30]. All parameters are extrapolated to infinite system sizes; see the SM [30].

Reconstr. from	to FH				to t - J		
	U/t	t_n/t	V/t	V'/t	J/t	t_3/t	V/t
HH	8.05				0.51	0.06	
	7.64		-0.64	-0.34	0.52	0.05	-0.44
Three-band FH	11.32	0.64			0.68	0.08	
	11.41	0.65	0.07		0.66	0.08	-0.02

2. Downfolding from the Emery model

To derive a single-band model from the three-band Fermi-Hubbard model, we adapt the down schemes from Refs. [6,40]: We start from the three-band model with two oxygen p_x and p_y sites and one copper d site. The goal is to define Wannier functions (WFs) centered on the copper sites and construct a matrix A out of them, defining a single-particle transformation from the three-band basis $\{C^\dagger\} = \{d^\dagger, p_x^\dagger, p_y^\dagger\}$ to the single-band (or WF) basis $\{c^\dagger\}$, $c_j^\dagger = \sum_j A_{ji} C_i^\dagger$. Following Ref. [6], we diagonalize the correlation matrix

$$M_{\alpha\beta} = \sum_{\sigma} \langle C_{\alpha\sigma}^\dagger C_{\beta\sigma} \rangle, \quad (10)$$

with $C^\dagger = \{d^\dagger, p_x^\dagger, p_y^\dagger\}$ to determine the natural orbitals $\{\psi_i\}$ of the interacting system. These $\{\psi_i\}$ can be centered around the copper sites by superposing them as follows:

$$\psi_j^C(\vec{r}) = \sum_i \psi_i(\vec{r} = \vec{r}_j) \psi_i(\vec{r}), \quad (11)$$

where $\vec{r}_j$ is the position vector corresponding to Cu site j . To also orthonormalize $\{\psi_j^C(\vec{r})\}$, we apply a minimal rotation denoted by $O_{jj'} = \langle \psi_j^C(\vec{r}) | \psi_{j'}^C(\vec{r}) \rangle$, yielding [6]

$$\psi_j^{CO}(\vec{r}) = \sum_j [O^{-\frac{1}{2}}]_{jj'} \psi_{j'}^C(\vec{r}_i). \quad (12)$$

A_{ji} is constructed from all $\psi_j^{CO}(\vec{r})$ for all j copper sites. The terms of the effective Hamiltonian can then be read off from the A -matrix [6,30].

3. Downfolding results

The reconstructed parameters are presented in Table I. For both original models, we find a strong on-site interaction $U \gg t$ in the single-band Fermi-Hubbard model, corresponding to a spin exchange of approximately $J/t \approx 0.5$. Additionally, the phononic description based on the Hubbard-Holstein model indeed yields an effective attraction in both the Fermi-Hubbard and t - J models, though its amplitude is smaller than anticipated for the ladder systems discussed above. In contrast, the protocol starting from the three-band model results in only a very weak density-density interaction,

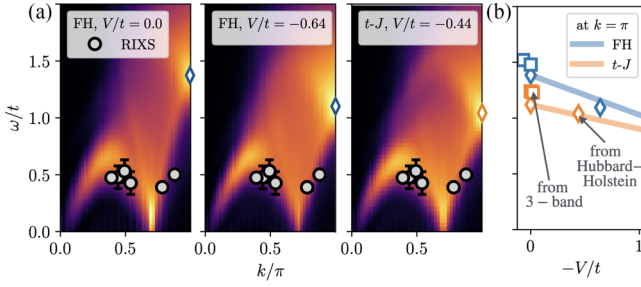


FIG. 3. Dynamical spin structure factor (DSF) for 1D compounds at 29% doping: (a) We compare RIXS measurements from Ref. [16] (circles) to the DSF for the Fermi-Hubbard model with $V/t = 0.0$, $V/t = -0.64$, and the t - J model with $V/t = -0.44$ (left to right color plots). Panel (b) shows how the energy of the peak at $k = \pi$ shifts downwards with $-V/t$ for both models. Squares represent the reconstruction from the three-band model, diamonds from the Hubbard-Holstein model; see Table I; lines are additional results with $V' = 0$ for reference.

which is even repulsive in the Fermi-Hubbard model. Instead, consistent with Ref. [6], we observe a strong density-assisted hopping term in the Fermi-Hubbard model,

$$\hat{\mathcal{H}}_n^{\text{kin}} = -t_n \sum_{(i,j)\sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.}) \hat{n}_{i\bar{\sigma}}. \quad (13)$$

The corresponding on-site repulsion looks stronger than usual at first glance, but when normalized to all hopping contributions $U/(t_n \langle n \rangle + t) \approx 8$, as usually considered. This renormalized hopping strength also explains the stronger J in the lower right part of Table I.

We now test the reconstructed single-band models—derived from the ground-states—by evaluating their performance on the DSF for hole doping $\delta = 29\%$. In the undoped case, the system exhibits a characteristic two-spinon continuum, analogous to that observed in ladder systems [41]. Upon doping, the gap-closing point shifts to $2k_F$, with k_F the Fermi momentum, and a spin gap opens at $k = \pi$. This is observed for $\delta = 29\%$ in Fig. 3(a) for all considered single-band models, including the bare Fermi-Hubbard model (left). However, a comparison with experimental RIXS measurements [10] and the theoretical predictions of the bare Fermi-Hubbard model shows a discrepancy of the DSF near the zone boundary: The spectral gap extends to higher energies than observed experimentally. As for the ladders, it was shown that the inclusion of an attraction $V = -t$ can decrease the spectral gap [23–25].

The Fermi-Hubbard and t - J reconstructions both feature attractive interactions, with again a smaller reconstructed $|V|$ for the t - J model than for the Fermi-Hubbard model, resulting in a similar trend for the DSF gap at $k = \pi$; see Fig. 3(a) (middle and right) and diamonds in Fig. 3(b). The reconstruction from the three-band model does not result in such a large attractive term, which in turn gives rise to a larger spectral gap, see squares in Fig. 3(b). In general, the gap is significantly lower for the t - J model. In particular, the gap of the t - J reconstruction with $V/t = -0.44$ is very close to the Fermi-Hubbard model with $V = -t$ that is considered in Refs. [23–25].

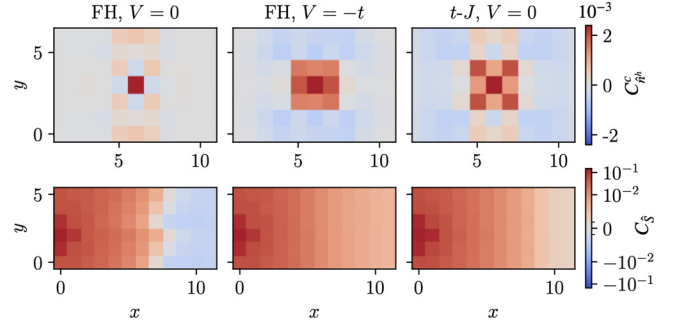


FIG. 4. Connected charge (top) and staggered spin (bottom) correlations for the Fermi-Hubbard model with $U/t = 8.0$ and $V/t = 0.0$, -1.0 (left, middle) and the t - J model with $J/t = 0.5$ and $V/t = 0.0$ (right) on cylinders (periodic boundaries in the y direction) with $L_x = 12$, $L_y = 6$ upon doping the half-filled system with two holes. For the Fermi-Hubbard model, the correlations are corrected for doublon-hole fluctuations.

As discussed in Ref. [24], additionally a softening of the spectral peak at $k = \pi$ and decreasing spectral weight at $2k_F$ is observed in both models when increasing $|V|$, which is in agreement with the theoretical DSF from the Hubbard-Holstein model. Again, we conclude that both Fermi-Hubbard and t - J models with similar attraction are in good agreement with the DSF from the experiment.

Note that similar results have been reported in angle-resolved ARPES studies [22,23,42]; however, the differences in the intensity of the holon-folding branch are much less pronounced (see the SM).

C. Two-dimensional systems

Finally, we turn to the two-dimensional case. To this end, we compare charge and spin correlation functions for cylinders of size $L_x = 12$, $L_y = 6$ upon doping the half-filled system with two holes. More specifically, we consider the connected density-density correlator for the holes

$$C_{\hat{n}^h}^c(\mathbf{i}, \mathbf{j}) = \langle \hat{n}_i^h \hat{n}_j^h \rangle - \frac{\langle \hat{N}^h \rangle - 1}{\langle \hat{N}^h \rangle} \langle \hat{n}_i^h \rangle \langle \hat{n}_j^h \rangle, \quad (14)$$

with the hole number operator $\hat{n}_i^h = (1 - \hat{n}_i^\uparrow)(1 - \hat{n}_i^\downarrow)$ and $\hat{N}^h = \sum_i \hat{n}_i^h$, and the normalization factor accounting for the finite number of holes in the system. We average this quantity over different reference sites along the periodic direction and, for the Fermi-Hubbard model, correct for doublon-hole fluctuations by subtracting the correlation function obtained from the ground-state with a single dopant hole [43]. Furthermore, we evaluate the staggered spin correlation function, defined as

$$C_S(\mathbf{i}) = (-1)^{\mathbf{i} \cdot \mathbf{i}_0} \langle \hat{S}_{(0,2)}^z \hat{S}_i^z \rangle, \quad (15)$$

with the reference site at position $(0,2)$ on the edge of the cylinder.

As shown in the top panel of Fig. 4, the charge correlations for the bare Fermi-Hubbard model exhibit anticorrelation for nearest neighbors and attractive features for next-nearest neighbors as well as along the periodic direction of the cylinder, indicating the formation of a stripe in the finite-size system. This is supported by a sign change in C_S (bottom

panel), consistent with the presence of a spin domain wall that accompanies the stripe. In contrast, for attractive interactions ($V = -t$), the stripe signal vanishes: strong pairing signatures appear in C_{ph}^c for both nearest and next-nearest neighbors, and the antiferromagnetic spin correlations extend across the entire system, without any domain wall. This behavior coincides with an increase in the binding energy from $E_B^{FH}(V = 0)/t = 0.10$ to $E_B^{FH}(V = -t)/t = 0.27$.

In the bare t - J model, similar pairing features are observed, along with an additional positive contribution from the stripe configuration, reminiscent of the behavior in the bare Fermi-Hubbard model. The antiferromagnetic spin correlations again span the entire system, as in the $FH + V$ case. The binding energy in this case, $E_B^{tJ}(V = 0)/t = 0.23$, is comparable to that of the Fermi-Hubbard model with attractive interactions.

II. CONCLUSIONS

In this work, we address the question of which minimal single-band model best captures the essential physics of cuprate superconductors, with a particular focus on extended versions of single-band Fermi-Hubbard and t - J models. We evaluate their suitability based on the magnetic excitation spectrum probed by the dynamical spin structure factor (DSF) and systematic ground-state reconstruction schemes.

Our key results are twofold: First, they suggest that for both single-band models, additional attractive terms, as suggested by recent experiments [8–10], can indeed be induced by phonons, while they do not occur in a reconstruction from the three-band model.

Second, we show that such a Fermi-Hubbard model with attractive interactions shares many properties with the t - J model—even without an explicit attractive interaction for the latter model—in chains, ladders, and two-dimensional systems. Most prominently, both $FH + V$ and the bare t - J

model are in agreement with recent RIXS measurements on cuprate ladder compounds, where a significant discrepancy between the experiment and the DSF from the bare Fermi-Hubbard model was found [8,9]. This can be attributed to the presence of strongly bound rung pairs in both $FH + V$ and bare t - J models.

Our results highlight both the need for further studies incorporating additional terms in single-band models and the remarkable agreement of the bare t - J model with experiments on cuprates resulting from the intrinsic strong pairing in this model.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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- [1] J. G. Bednorz and K. A. Müller, Possible high T_c superconductivity in the Ba-La-Cu-O system, *Z. Phys. B* **64**, 189 (1986).
 - [2] V. J. Emery, Theory of high- T_c superconductivity in oxides, *Phys. Rev. Lett.* **58**, 2794 (1987).
 - [3] C. Weber, K. Haule, and G. Kotliar, Apical oxygens and correlation strength in electron- and hole-doped copper oxides, *Phys. Rev. B* **82**, 125107 (2010).
 - [4] C. Weber, C. Yee, K. Haule, and G. Kotliar, Scaling of the transition temperature of hole-doped cuprate superconductors with the charge-transfer energy, *Europhys. Lett.* **100**, 37001 (2012).
 - [5] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions, *Rev. Mod. Phys.* **68**, 13 (1996).
 - [6] S. Jiang, D. J. Scalapino, and S. R. White, Density matrix renormalization group based downfolding of the three-band Hubbard model: Importance of density-assisted hopping, *Phys. Rev. B* **108**, L161111 (2023).
 - [7] H. Xu, C.-M. Chung, M. Qin, U. Schollwöck, S. R. White, and S. Zhang, Coexistence of superconductivity with partially filled stripes in the Hubbard model, *Science* **384**, eadh7691 (2024).
 - [8] H. Padma, J. Thomas, S. F. R. TenHuisen, W. He, Z. Guan, J. Li, B. Lee, Y. Wang, S. H. Lee, Z. Mao, H. Jang, V. Bisogni, J. Pellicciari, M. P. Mark Dean, S. Johnston, and M. Mitrano, Beyond-Hubbard pairing in a cuprate ladder, *Phys. Rev. X* **15**, 021049 (2025).
 - [9] A. Scheie, P. Laurell, J. Thomas, V. Sharma, A. I. Kolesnikov, G. E. Granroth, Q. Zhang, B. Lake, M. Mihalik, Jr., R. I. Bewley, R. S. Eccleston, J. Akimitsu, E. Dagotto, C. D. Batista, G. Alvarez, S. Johnston, and D. A. Tennant, Cooper-pair localization in the magnetic dynamics of a cuprate ladder, *arXiv:2501.10296*.
 - [10] J. Li, D. Jost, T. Tang, R. Wang, Y. Zhong, Z. Chen, M. Garcia-Fernandez, J. Pellicciari, V. Bisogni, B. Moritz, K. Zhou, Y. Wang, T. P. Devereaux, W.-S. Lee, and Z.-X. Shen, Doping dependence of 2-spinon excitations in the doped 1D cuprate $\text{Ba}_2\text{CuO}_{3+\delta}$, *Phys. Rev. Lett.* **134**, 146501 (2025).
 - [11] F. C. Zhang and T. M. Rice, Effective Hamiltonian for the superconducting Cu oxides, *Phys. Rev. B* **37**, 3759 (1988).

- [12] C. Ye, P. Cai, R. Yu, X. Zhou, W. Ruan, Q. Liu, C. Jin, and Y. Wang, Visualizing the atomic-scale electronic structure of the $\text{Ca}_2\text{CuO}_2\text{Cl}_2$ Mott insulator, *Nat. Commun.* **4**, 1365 (2013).
- [13] S. Ye, J. Zhao, Z. Yao, S. Chen, Z. Dong, X. Li, L. Shi, Q. Liu, C. Jin, and Y. Wang, Visualizing the Zhang-Rice singlet, molecular orbitals and pair formation in cuprate, [arXiv:2309.09260](https://arxiv.org/abs/2309.09260).
- [14] L. H. Tjeng, B. Sinkovic, N. B. Brookes, J. B. Goedkoop, R. Hesper, E. Pellegrin, F. M. F. de Groot, S. Altieri, S. L. Hulbert, E. Shekel, and G. A. Sawatzky, Spin-resolved photoemission on anti-ferromagnets: Direct observation of Zhang-Rice singlets in CuO , *Phys. Rev. Lett.* **78**, 1126 (1997).
- [15] Y. Harada, K. Okada, R. Eguchi, A. Kotani, H. Takagi, T. Takeuchi, and S. Shin, Unique identification of Zhang-Rice singlet excitation in $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ mediated by the O $1s$ core hole: Symmetry-selective resonant soft x-ray Raman scattering study, *Phys. Rev. B* **66**, 165104 (2002).
- [16] S. Li, A. Nocera, U. Kumar, and S. Johnston, Particle-hole asymmetry in the dynamical spin and charge responses of corner-shared 1D cuprates, *Commun. Phys.* **4**, 217 (2021).
- [17] H.-B. Schüttler and A. J. Fedro, Copper-oxygen charge excitations and the effective-single-band theory of cuprate superconductors, *Phys. Rev. B* **45**, 7588 (1992).
- [18] J. H. Jefferson, H. Eskes, and L. F. Feiner, Derivation of a single-band model for CuO_2 planes by a cell-perturbation method, *Phys. Rev. B* **45**, 7959 (1992).
- [19] V. I. Belinicher and A. L. Chernyshev, Reduction of a three-band model for copper oxides to a single-band generalized t - J model, *Phys. Rev. B* **47**, 390 (1993).
- [20] V. I. Belinicher, A. L. Chernyshev, and L. V. Popovich, Range of the t - J model parameters for CuO_2 planes: Experimental data constraints, *Phys. Rev. B* **50**, 13768 (1994).
- [21] L. F. Feiner, J. H. Jefferson, and R. Raimondi, Effective single-band models for the high- T_c cuprates. I. Coulomb interactions, *Phys. Rev. B* **53**, 8751 (1996).
- [22] A. E. Feiguin, C. Helman, and A. A. Aligia, Effective one-band models for the one-dimensional cuprate $\text{Ba}_{2-x}\text{Sr}_x\text{CuO}_{3+\delta}$, *Phys. Rev. B* **108**, 075125 (2023).
- [23] T. Tohyama, H. Maeda, K. Tsutsui, S. Sota, and S. Yunoki, Spin and charge dynamics of doped one-dimensional Mott insulators, *Phys. Rev. B* **110**, 125106 (2024).
- [24] T. Tang, D. Jost, B. Moritz, and T. P. Devereaux, Influence of extended interactions on spin dynamics in one-dimensional cuprates, *Phys. Rev. B* **110**, 165118 (2024).
- [25] Z. Shen, J. Liu, H.-X. Wang, and Y. Wang, Signatures of the attractive interaction in spin spectra of one-dimensional cuprate chains, *Phys. Rev. Res.* **6**, L032068 (2024).
- [26] Z. Chen, Y. Wang, S. N. Rebec, T. Jia, M. Hashimoto, D. Lu, B. Moritz, R. G. Moore, T. P. Devereaux, and Z.-X. Shen, Anomalous strong near-neighbor attraction in doped 1D cuprate chains, *Science* **373**, 1235 (2021).
- [27] Y. Wang, Z. Chen, T. Shi, B. Moritz, Z.-X. Shen, and T. P. Devereaux, Phonon-mediated long-range attractive interaction in one-dimensional cuprates, *Phys. Rev. Lett.* **127**, 197003 (2021).
- [28] X.-L. Qi and D. Ranard, Determining a local Hamiltonian from a single eigenstate, *Quantum* **3**, 159 (2019).
- [29] T. Barnes, E. Dagotto, J. Riera, and E. S. Swanson, Excitation spectrum of Heisenberg spin ladders, *Phys. Rev. B* **47**, 3196 (1993).
- [30] See Supplemental Material at <https://link.aps.org/supplemental/10.1103/n2ql-32n3> for additional information on the numerical calculations, the reconstruction schemes and comparisons of the reconstruction from the Hubbard-Holstein model to a Lang-Firsov transformation.
- [31] T. Köhler, J. Stolpp, and S. Paeckel, Efficient and flexible approach to simulate low-dimensional quantum lattice models with large local Hilbert spaces, *SciPost Phys.* **10**, 058 (2021).
- [32] S. Singh, R. N. C. Pfeifer, and G. Vidal, Tensor network states and algorithms in the presence of a global $U(1)$ symmetry, *Phys. Rev. B* **83**, 115125 (2011).
- [33] S. Paeckel, T. Köhler, and S. R. Manmana, Automated construction of $U(1)$ -invariant matrix-product operators from graph representations, *SciPost Phys.* **3**, 035 (2017).
- [34] S. Paeckel, T. Köhler, A. Swoboda, S. R. Manmana, U. Schollwöck, and C. Hubig, Time-evolution methods for matrix-product states, *Ann. Phys.* **411**, 167998 (2019).
- [35] T. Barthel, U. Schollwöck, and S. R. White, Spectral functions in one-dimensional quantum systems at finite temperature using the density matrix renormalization group, *Phys. Rev. B* **79**, 245101 (2009).
- [36] Z. Zhou, W. Ye, H.-G. Luo, J. Zhao, and J. Chang, Robust superconducting correlation against intersite interactions in the extended two-leg Hubbard ladder, *Phys. Rev. B* **108**, 195136 (2023).
- [37] H. Tsunetsugu, M. Troyer, and T. M. Rice, Pairing and excitation spectrum in doped t - J ladders, *Phys. Rev. B* **49**, 16078 (1994).
- [38] S. R. White and D. J. Scalapino, Hole and pair structures in the t - J model, *Phys. Rev. B* **55**, 6504 (1997).
- [39] B. K. Chakraverty, J. Ranninger, and D. Feinberg, Experimental and theoretical constraints of bipolaronic superconductivity in high T_c materials: An impossibility, *Phys. Rev. Lett.* **81**, 433 (1998).
- [40] R. C. Sawaya and S. R. White, Constructing Hubbard models for the hydrogen chain using sliced-basis density matrix renormalization group, *Phys. Rev. B* **105**, 045145 (2022).
- [41] J. des Cloizeaux and J. J. Pearson, Spin-wave spectrum of the antiferromagnetic linear chain, *Phys. Rev.* **128**, 2131 (1962).
- [42] T. Tang, B. Moritz, C. Peng, Z.-X. Shen, and T. P. Devereaux, Traces of electron-phonon coupling in one-dimensional cuprates, *Nat. Commun.* **14**, 3129 (2023).
- [43] T. Blatz, U. Schollwöck, F. Grusdt, and A. Bohrdt, Two-dopant origin of competing stripe and pair formation in Hubbard and t - J models, *Phys. Rev. X* **15**, 031074 (2025).