

# Extended $s$ -wave pairing from an emergent Feshbach resonance in bilayer nickelate superconductors

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Since the discovery of unconventional superconductivity in cuprates, unraveling the pairing mechanism of charge carriers in doped antiferromagnets has been a long-standing challenge. Motivated by the discovery of high- $T_c$  superconductivity in nickelate bilayer  $\text{La}_3\text{Ni}_2\text{O}_7$  (LNO), we study a minimal mixed dimensional  $t - J$  model supplemented with a repulsive Coulomb interaction  $V$ . When hole doped, previous numerical simulations revealed that the system exhibits strong binding energies, with a phenomenology resembling a BCS-to-BEC crossover accompanied by a Feshbach resonance between two distinct types of charge carriers. Here, we perform a mean-field analysis that enables a direct observation of the BCS-to-BEC crossover as well as microscopic insights into the crossover region and the pairing symmetry for two-dimensional bilayers. We benchmark our mean-field description by comparing it to density-matrix renormalization group simulations in quasi-one-dimensional settings and find remarkably good agreement. For the two-dimensional system relevant to LNO, our mean-field calculations predict a BCS pairing gap with an extended  $s$ -wave symmetry, directly resulting from the pairing mechanism's Feshbach origin. Our analysis hence gives insights into pairing in unconventional superconductors and, further, can be tested in currently available ultracold atom experiments.

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Starting with the discovery of superconductivity in cuprate materials about four decades ago [1–4], the search for superconductors with high critical temperatures has revealed unconventional superconductivity in various materials, including nickelate and cuprate compounds [5,6]. Recently, the bilayer nickelate  $\text{La}_3\text{Ni}_2\text{O}_7$  (LNO) was observed to become superconducting under pressure at a critical temperature of 80K [7–9], with a pairing gap of extended  $s$ -wave symmetry predicted by theoretical works [10–13], similar to those in infinite layer nickelates [14], iron-based superconductors [15], and the strongly coupled bilayer Hubbard model [16–18]. Following the observation of high- $T_c$  superconductivity in LNO, theoretical studies suggested that a minimal effective low-energy model that governs the physics of these materials is a mixed dimensional (MixD) bilayer  $t - J$  model, i.e., a single band  $t - J$  model with suppressed inter-layer hopping but strong antiferromagnetic coupling between the layers (see Fig. 1) [19–22]. More realistic multiorbital models have also been proposed [21,23,24]. To find a minimal description for nickelate superconductors, investigating the pairing mechanism in MixD  $t - J$  bilayers represents a crucial step toward developing a microscopic understanding of pairing in

these unconventional superconductors. However, the nature of pairing and the pairing symmetry within this model remain elusive.

Since in contrast to conventional superconductors, high- $T_c$  superconductors feature significant pairing gaps, i.e., smaller Cooper pairs which possibly experience repulsive Coulomb interactions, the Coulomb repulsion  $V$  is typically not negligible in these materials [25]. We account for that with an additional nearest-neighbor repulsion  $V$  between holes on the same rung of the bilayer. While this formulation is directly inspired by bilayer nickelates, the resulting MixD  $t - J + V$  model also serves as a minimal platform to explore pairing in presence of strong correlations and short-range repulsion. Its mixed-dimensional structure and tunable interactions make it particularly suitable for implementation in ultracold atom systems, where key parameters can be engineered with high precision [26]. Thus, our choice of parameters is not meant as a literal fit for LNO but rather as an illustration of the pairing mechanism and pairing features of a minimal model in connection to the bilayer nickelate compounds. These MixD  $+ V$  systems have been shown to host the following emergent structures upon doping the ground state at half filling, consisting of singlets on each rung of the ladder [25–30]: (i) at small  $V/J_\perp$  two holes form a tightly bound state of two chargons [chargon( $c$ )-chargon( $c$ ) pair,  $cc$ 's] with strong binding energy. This is the result of interlayer exchange  $J_\perp$  and coherent movement of the  $cc$ 's through the system in order to minimize distortions of the (antiferromagnetic) AFM background [28]. (ii) At large  $V/J_\perp$  the system is dominated by spatially extended pairs of two partons, a spinon and

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a chargon [spinon(*s*)-chargon(*c*) pair, *sc*'s]. In between (i) and (ii), a crossover from a Bose-Einstein condensate (BEC) of *cc*'s to a strongly correlated Bardeen–Cooper–Schrieffer (BCS) regime with pairs of *sc*'s (*sc*<sup>2</sup>) is observed [23,25], which features a pairing dome with relatively high binding energy [30]. Each *sc*<sup>2</sup> is thus composed of two mesons (*sc*'s), comprising a total of four partons: two chargons and two spinons.

While binding between holes in the *cc*'s can be explained with kinetic arguments, making it favorable for holes to move together through the system [27,28], binding of pairs of *sc*'s into *sc*<sup>2</sup> originates from a more subtle mechanism, leading to more spatially extended Cooper pairs of holes [25,30]: In the BCS regime, where *sc*'s govern the low-energy physics, numerical and analytical results suggest that binding is mediated via couplings to the high-energy *cc* channel, resembling a Feshbach resonance between the low-energy (open) *sc* channel and the high-energy (closed) *cc* channel. This Feshbach mediated pairing mechanism [31,32] features many similarities to the phenomenology of bilayer nickelate but also cuprate superconductors [25,29,30]: (i) Pairing is facilitated by doping, leading to a dome of binding energies with its peak at intermediate doping. (ii) Pairing only requires short-range antiferromagnetic (AFM) correlations but no long-range magnetic order. (iii) The Fermi surface volume changes [24], similar to the small-to-large Fermi surface transition in cuprates. (iv) For single-layer models, the resulting pairing gap is predicted to have the *d*-wave symmetry observed in cuprates [31], and, as we will show here, for bilayers the extended *s*-wave symmetry predicted for LNO can be explained. So far, these observations have been made by comparing effective theories in terms of the emergent constituents and numerical observations in single and coupled ladders deep in the *cc*'s and *sc*<sup>2</sup> regimes. However, a description of the intermediate regime where *sc*<sup>2</sup> and *cc* hybridize, needed to fully test the prediction of Feshbach mediated pairing, is lacking.

Here, we go beyond earlier analysis and derive an effective mean-field (MF) description of the *sc* and *cc* constituents in the intermediate regime that captures the essential physics of the BCS-to-BEC crossover and of the Feshbach resonance. We compare our mean-field predictions to density matrix renormalization group (DMRG) simulations of the MixD + *V* ladder to validate the model. To further support the extension of the mean-field approach to higher dimensions we also perform the comparison for the quasi-2D two-ladder system, see Fig. 4. Then, we apply our analysis to the 2D systems relevant to LNO. Our analysis allows us to understand the BCS-to-BEC crossover in terms of the corresponding order parameters. Furthermore, it reveals the extended *s*-wave symmetry of the pairing gap as a direct consequence of the Feshbach mediated pairing mechanism; see Fig. 2.

## I. MICROSCOPIC MODEL

The MixD *t* – *J* bilayer supplemented with a repulsive interaction *V* was first introduced in Refs. [23,25,30]. It features nearest-neighbor hopping with amplitude *t*<sub>∥</sub>, superexchange interaction *J*<sub>⊥</sub> and repulsive Coulomb interaction *V* between

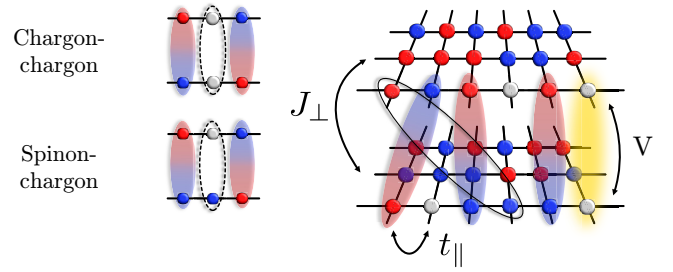


FIG. 1. Schematic depiction of the 2D MixD + *V* bilayer model (right) and its quasi-particle constituents (left). We highlight the emergent constituents that characterize the two sides of the BCS-to-BEC crossover existing in this system: on the BCS side the system is dominated by spatially extended pairs (*sc*<sup>2</sup>) of spinon-chargeons (*sc*'s), involving one extended singlet (highlighted in the figure). The BEC side features tightly bound chargeon-chargeons (*cc*'s) characterized by the Coulomb repulsion *V* (yellow shadow).

holes on the same rung, i.e.,

$$\hat{\mathcal{H}} = -t_{\parallel} \hat{\mathcal{P}} \sum_j \sum_{\mu, \sigma} (\hat{c}_{j+1\mu\sigma}^{\dagger} \hat{c}_{j\mu\sigma} + \text{H.c.}) \hat{\mathcal{P}} + J_{\perp} \sum_j \left( \hat{\mathbf{S}}_{j0} \cdot \hat{\mathbf{S}}_{j1} - \frac{1}{4} \hat{n}_{j0} \hat{n}_{j1} \right) + V \sum_j \hat{n}_{j0}^h \hat{n}_{j1}^h. \quad (1)$$

Here,  $\hat{\mathcal{P}}$  is the Gutzwiller projector onto the subspace with maximum single occupancy per site. Spin and density operators at site *j* and layer  $\mu = 0, 1$  are represented by  $\hat{\mathbf{S}}_{j\mu}$  and  $\hat{n}_{j\mu} = \hat{n}_{j\mu\uparrow} + \hat{n}_{j\mu\downarrow}$ . The hole density operators are denoted by  $\hat{n}_{j\mu}^h = 1 - \hat{n}_{j\mu}$ .

The motivation for studying the MixD + *V* model is twofold: First, the recently discovered bilayer nickelate La<sub>3</sub>Ni<sub>2</sub>O<sub>7</sub>, showing superconducting behavior with *T*<sub>c</sub> = 80 K under high pressure, effectively realizes a bilayer MixD *t* – *J* model. This can be seen from DFT calculations that reveal that the low-energy degrees of freedom are the 3*d*<sub>z<sup>2</sup></sub> and 3*d*<sub>x<sup>2</sup>–y<sup>2</sup></sub> Ni orbitals [20], featuring strong Hund's coupling between them. The *d*<sub>z<sup>2</sup></sub> orbitals induce interlayer AFM superexchange interactions via the O-2*p* orbitals in the intercalated LaO layer.

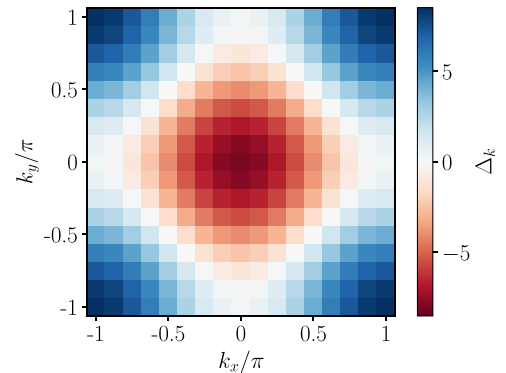


FIG. 2. In the crossover regime, the spinon-chargeon pairs are described by the BCS wave function. Here we consider a 2D MixD + *V* model on a 16 × 16 square lattice with  $\frac{t_{\parallel}}{V} = 0.1$ ,  $J_{\perp} = V$  and  $\delta = \frac{128}{256}$  holes in the system. The figure shows the value of the BCS order parameter  $\Delta_k$  realizing an extended *s*-wave pairing symmetry.

In contrast, the  $d_{x^2-y^2}$  orbitals are responsible for a weak intralayer hopping  $t_{\parallel}$  and AFM coupling  $J_{\parallel}$ . In the limit of large Hund's coupling between the two  $3d$  orbitals, the system realizes an effective AFM interaction  $J_{\perp}$  between the two layers, and the interlayer hopping  $t_{\perp}$  is suppressed [20]. Moreover, as stated before, we need to account for the Coulomb repulsion  $V$  between neighboring holes, arising from the limited spatial extension of Cooper pairs in unconventional superconductors. The second motivation to study the MixD +  $V$  model is their realizability in cold atom experiments: In Ref. [26], a MixD ladder was realized by applying a potential offset between the legs of the ladder, effectively enhancing  $J_{\perp}$  and suppressing the perpendicular hopping [26–28]. This system can be supplemented with nearest-neighbor repulsion by doping one leg with doublons and one with holes, see Refs. [25,30,33].

The ground state of this MixD +  $V$  model at zero doping consists of one singlet on each rung of the ladder [27,28]. At finite doping, the physics of the system is determined by the competition between the kinetic energy of the holes and the energy from the distortion of the magnetic background due to the motion of the holes. In the tight-binding regime  $t_{\parallel} \ll J_{\perp}, V$ , the emerging constituents can be easily understood in the following two limits: When  $J_{\perp} \gg V$ , the low-energy constituents of the system are  $cc$ 's, minimizing the distortion of the spin background. On the contrary, for  $J_{\perp} \ll V$ , each rung will tend to be occupied at maximum by one hole (and one spin), forming a spinon-chargon. In this regime, both emergent charge carriers can be assumed point-like, i.e., with constituents on the same rung [25,28]. In previous works [25,30], it was shown that the transition between the two limits can be explained as a crossover associated with a Feshbach resonance from tightly bound pairs of holes (closed channel) at small repulsion to more spatially extended, correlated pairs of individual holes (open channel) at large repulsion [31]. In this picture, attractive interactions in the open channel are mediated by processes that couple to the closed channel even for large repulsion  $V > J_{\perp}, t_{\parallel}$ .

## II. MEAN-FIELD THEORY

Earlier studies [25,30] provided a qualitative understanding of the physics of the MixD +  $V$  model in the limiting cases where either  $sc$ 's (large  $V/J_{\perp}$ ) or  $cc$ 's (small  $V/J_{\perp}$ ) are dominant in the system, but the exploration of the crossover regime  $J_{\perp} \approx V$  was limited to DMRG simulations of single and a few coupled ladders. Furthermore, such numerical methods do not directly provide access to the pairing gap. In contrast, here we obtain microscopic insight into the physics of the MixD +  $V$  model in the crossover regime where both  $cc$ 's and  $sc$ 's are present: We derive an effective two-channel Hamiltonian in terms of  $sc$ 's  $f_{j\mu\sigma}^{(\dagger)}$  and  $cc$ 's  $b_j^{(\dagger)}$  by performing a Schrieffer-Wolff transformation of Eq. (1), assuming

$$t_{\parallel} \ll J_{\perp}, V, \quad (2)$$

hence pointlike  $sc$ 's and  $cc$ 's. Then, we develop a MF theory to solve the resulting model.

In this limit, both  $sc$ 's and  $cc$ 's belong to the low-energy manifold, whereas the high-energy subspace contains con-

figurations comprised of distorted singlets. The effective Hamiltonian we obtain reads

$$\hat{\mathcal{H}}_{\text{eff}}^{sc,cc} = \hat{\mathcal{H}}_{\text{kin}}^{sc} + \hat{\mathcal{H}}_{\text{pot}}^{sc} + \hat{\mathcal{H}}_{\text{pot}}^{cc} + \hat{\mathcal{H}}_{\text{int}}^{sc,sc} + \hat{\mathcal{H}}_{\text{rec}}^{sc,cc} + \mu_h(\hat{N}_f + \hat{N}_b - N_h), \quad (3)$$

$$\hat{\mathcal{H}}_{\text{kin}}^{sc} = + \frac{t_{\parallel}}{2} \sum_{\langle i,j \rangle} \sum_{\mu\sigma} \hat{\mathcal{P}}_f (\hat{f}_{i\mu\sigma}^{\dagger} \hat{f}_{j\mu\sigma} + \text{H.c.}) \hat{\mathcal{P}}_f - t_{\parallel} \sum_{\langle i,j \rangle} \sum_{\mu\sigma} \hat{\mathcal{P}}_f (\hat{f}_{i\mu\sigma}^{\dagger} \hat{b}_j^{\dagger} \hat{b}_i \hat{f}_{j\mu\sigma} + \text{H.c.}) \hat{\mathcal{P}}_f, \quad (4)$$

$$\hat{\mathcal{H}}_{\text{pot}}^{sc} = \left( J_{\perp} - \frac{3}{2} \frac{t_{\parallel}^2}{J_{\perp}} \right) \sum_{j\mu} \hat{n}_{j\mu}^f, \quad (5)$$

$$\hat{\mathcal{H}}_{\text{pot}}^{cc} = (V + J_{\perp}) \sum_i \hat{b}_i^{\dagger} \hat{b}_i, \quad (6)$$

$$\hat{\mathcal{H}}_{\text{int}}^{sc,sc} = + \frac{3}{2} \frac{t_{\parallel}^2}{J_{\perp}} \sum_{\langle i,j \rangle} \sum_{\mu\mu'} \hat{n}_{i\mu}^f \hat{n}_{j\mu'}^f - 4 \frac{t_{\parallel}^2}{V} \sum_{\langle i,j \rangle} \left( -\hat{\mathbf{J}}_i \cdot \hat{\mathbf{J}}_j + \frac{1}{4} \right) \left( \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + \frac{3}{4} \hat{n}_i^f \hat{n}_j^f \right), \quad (7)$$

$$\hat{\mathcal{H}}_{\text{rec}}^{sc,cc} = - \frac{t_{\parallel}}{\sqrt{2}} \sum_{\langle i,j \rangle} \sum_{\mu,\sigma} (-1)^{\sigma} \hat{\mathcal{P}}_f (\hat{f}_{i\mu\sigma}^{\dagger} \hat{f}_{j\bar{\mu}\bar{\sigma}}^{\dagger} \hat{b}_j + \text{H.c.}) \hat{\mathcal{P}}_f, \quad (8)$$

where Eq. (4) corresponds to the kinetic energy of the  $sc$ 's and  $cc$ 's, and Eqs. (5) and (6) are respectively the terms associated with the  $sc$ 's and the  $cc$ 's chemical potential. The term in Eq. (7) takes into account the interactions between  $sc$ 's sitting on neighboring rungs, which are subject to repulsive interaction  $\propto +\frac{3}{2} \frac{t_{\parallel}^2}{J_{\perp}}$  and attractive interaction  $\propto \frac{t_{\parallel}^2}{V}$  for triplet states. The term in Eq. (8) describes the recombination of a pair of two neighboring  $sc$ 's (open channel) into one  $cc$  (closed channel) and vice versa, giving rise to the Feshbach resonance as the presence of  $cc$ 's lowers the energy of the  $sc$  channel. The last term  $\propto \mu_h$  fixes the total number of holes in the system. In the above,  $\hat{n}_{j\mu}^f = \hat{n}_{j\mu\uparrow}^f + \hat{n}_{j\mu\downarrow}^f$  denotes the  $sc$ 's density while the layer-isospin operator  $\hat{\mathbf{J}}_i$  and the spin operator  $\hat{\mathbf{S}}_i$  are defined in the Supplemental Material [34]. To capture the low-energy physics of  $(sc)^2$ -to- $cc$  crossover, we consider the following ansatz for the ground state wave function:

$$|\Psi\rangle = \left[ \prod_k \left( u_k + v_k \frac{1}{\sqrt{2}} \sum_{\sigma} (-1)^{\sigma} \hat{f}_{k\mu\sigma}^{\dagger} \hat{f}_{-k\bar{\mu}\bar{\sigma}}^{\dagger} \right) \otimes \mathcal{N} \exp(\beta \hat{b}_{k=0}^{\dagger}) \right] |0\rangle, \quad (9)$$

where the first term accounts for the BCS pairing of  $sc$ 's with variational parameters  $u_k, v_k \in \mathbb{C}$ . The explicit singlet structure of the  $sc$ 's (note that  $\bar{\sigma}$  and  $\bar{\mu}$  denote the respective opposite spin and layer) is motivated by the fact that for sufficiently large  $V$  holes on the same rung strongly repel each other due to Coulomb interaction. Therefore, as  $\frac{J_{\perp}}{V}$  is decreased, the  $cc$ 's are disrupted and the displacement of the two holes constituting the  $cc$  leads to the formation of a tilted singlet between two neighboring spinons on opposite layers.

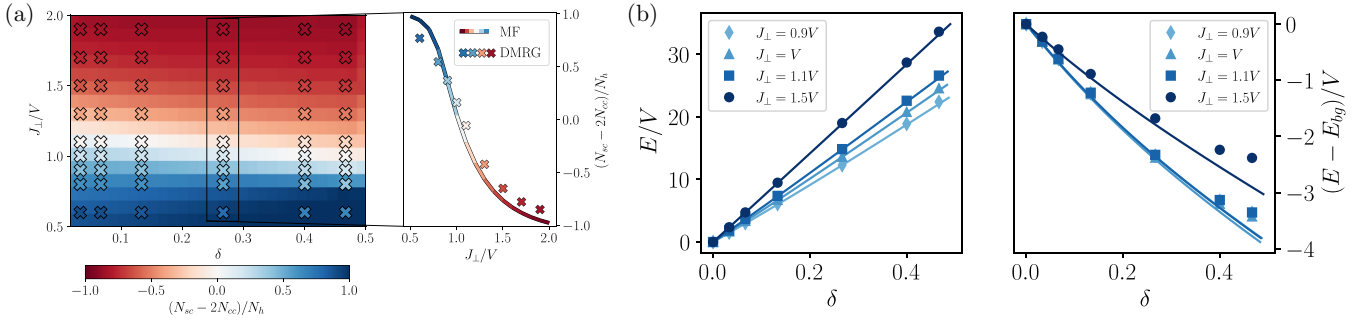


FIG. 3. Quasiparticle densities and ground state energy for the doped 1D ladder. (a) We compare the  $sc$  and  $cc$  densities for a 1D ladder as the ratio  $\frac{J_{\perp}}{V}$  and the doping  $\delta$  are tuned. We compute  $(N_{sc} - 2N_{cc})/N_h$ , where  $N_{sc}$  and  $N_{cc}$  are, respectively, the number of  $sc$ 's and  $cc$ 's in the system as defined in Sec. III;  $N_h$  is the total number of holes. This allows to distinguish the two sides of the crossover. The inset shows the section at constant doping  $\delta = \frac{8}{30}$  with the corresponding colors. We find good agreement between DMRG (crosses) and mean-field (color plot/solid line) for a MixD + V ladder of size  $L = 30$ , where we have fixed  $\frac{t_{\parallel}}{V} = 0.1$ . (b) The ground state energy  $E$  (left) of the microscopic model for a 1D ladder system from DMRG (markers) is reproduced well by the mean-field prediction for the effective Hamiltonian (solid lines). The agreement is also good for the ground state energies without considering the contribution from the background distortion  $E - E_{bg} = E - J_{\perp}N_{sc} - (V + J_{\perp})N_{cc}$  (right).

The second term describes the BEC of tightly bound  $cc$ 's with normalization constant  $\mathcal{N}$  and order parameter  $\beta \in \mathbb{C}$ . Here,  $|0\rangle$  denotes the  $sc$ 's and  $cc$ 's vacuum state, consisting of singlets on each rung. Our goal in the following is to tune  $\frac{J_{\perp}}{V}$  to transition from the BEC regime of tightly bound  $cc$ 's, where we expect large  $\beta$ , to the BCS regime where the  $sc$ 's form extended Cooper pairs in a BCS state. At the resonance, between the two regimes, the effective  $sc$  scattering length diverges. To describe this intermediate regime, it is important to include explicitly the coupling between the two channels ( $sc$  and  $cc$ ).

By minimizing the energy expectation value of the Hamiltonian in Eq. (3) with respect to the variational parameters of the wave function in Eq. (9),  $\partial_{u_k v_k} \partial_{\beta} \langle \Psi | \hat{\mathcal{H}}_{\text{eff}}^{sc,cc} | \Psi \rangle = 0$ , see Supplemental Material [34] (including Refs. [35]), we obtain the ground state properties of the system. To analytically perform the mean-field calculations, we neglect the Gutzwiller projections in Eq. (3). This is expected to be a good approximation for low doping and we restrict our analysis to values of the hole doping  $\delta < 0.5$ .

### III. BENCHMARKING MEAN-FIELD IN 1D MIXD + V LADDERS

We compare the results from our mean-field analysis with DMRG simulations, obtained using the package SYTEN with particle conservation in each leg and a global  $U(1)_{S_z}$  symmetry [36–38]. In Fig. 3, we focus on 1D ladder systems where the  $sc$ 's and  $cc$ 's densities of the microscopic model of Eq. (1) computed with DMRG are compared to the ground state mean-field results obtained from the effective Hamiltonian in Eq. (3). In particular, the difference between the number of holes contributing to the  $sc$ 's sector and  $cc$ 's sector  $\propto N_{sc} - 2N_{cc}$  is shown as a function of  $\frac{J_{\perp}}{V}$  and hole doping  $\delta$ . The two different regimes can be identified by the change in sign of the above quantity. Here,  $\hat{n}_{cc} = \frac{1}{L} \sum_i \hat{n}_{i\mu=1}^h \hat{n}_{i\mu=0}^h$  and  $\hat{n}_{sc} = \frac{1}{L} \sum_i \hat{n}_{i\mu=1}^h (1 - \hat{n}_{i\mu=0}^h)$  for the microscopic model, and  $\hat{n}_{cc} = \frac{1}{L} \sum_i \hat{b}_i^{\dagger} \hat{b}_i$  and  $\hat{n}_{sc} = \frac{1}{L} \sum_{i\mu} \hat{n}_{i\mu}^f$  for the MF theory.

As for the MF calculations, both species are considered to be pointlike since the system is probed in the tight binding regime  $t_{\parallel} \ll J_{\perp}, V$ . We find that for  $V > J_{\perp}$  the system is dominated by  $sc$ 's and the number of  $cc$ 's is negligible. For lower doping, however, it is expected to grow linearly for  $\delta > 0.5$  due to the single occupancy restriction [25], which we cannot capture within MF theory. For  $V < J_{\perp}$  the formation of  $sc$ 's is suppressed and the holes are bound together in  $cc$ 's. Fig. 3(a) compares the ground state energy obtained from DMRG and MF theory for different values of  $\frac{J_{\perp}}{V}$  at low doping. In the tight binding regime, when the system is hole doped, a large contribution to the ground state energy comes from the distortion of the AFM background:  $J_{\perp}N_{sc}$  for the  $sc$ 's and  $(V + J_{\perp})N_{cc}$  for the  $cc$ 's. However, the role of the kinetic, interaction, and recombination terms is not negligible; this is shown in Fig. 3(b), where we compare the ground state energies after subtracting the  $sc$ 's and  $cc$ 's background terms mentioned above. We also extend the analysis to the quasi-2D two-ladder system and report the results in Fig. 4. In both cases, there is good agreement, validating our MF approach.

Next, we calculate the binding energies, defined as

$$E_B(N_h) = 2(E_{N_h-2} - E_{N_h-1}) - (E_{N_h-2} - E_{N_h}), \quad (10)$$

where  $N_h$  is the number of holes in the system, added alternately to each layer. The expression can be evaluated directly from the DMRG ground state energies at different doping. For the mean-field theory, we obtain the binding energy by computing the terms in Eq. (10) separately. We consider the system in the BEC regime; here, the addition of two holes leads to the formation of a  $cc$  and  $E_{N_h-2} - E_{N_h} \approx 0$  since the energy required to add a quasiparticle to the condensate is approximately zero. However, the addition of one single hole corresponds to the creation of a single quasiparticle in the BCS state, which leads to an energy variation of  $E_{N_h-1} - E_{N_h} = \min_k (E_k)$  with  $E_k = \sqrt{\Delta_k^2 + \xi_k^2}$ , where  $\Delta_k$  is the BCS order parameter and  $\xi_k$  is the dispersion relation for  $sc$ 's; see Supplemental Material [34]. Therefore, the binding energies are given by  $E_B = 2(E_{N_h-2} - E_{N_h-1}) - (E_{N_h-2} -$

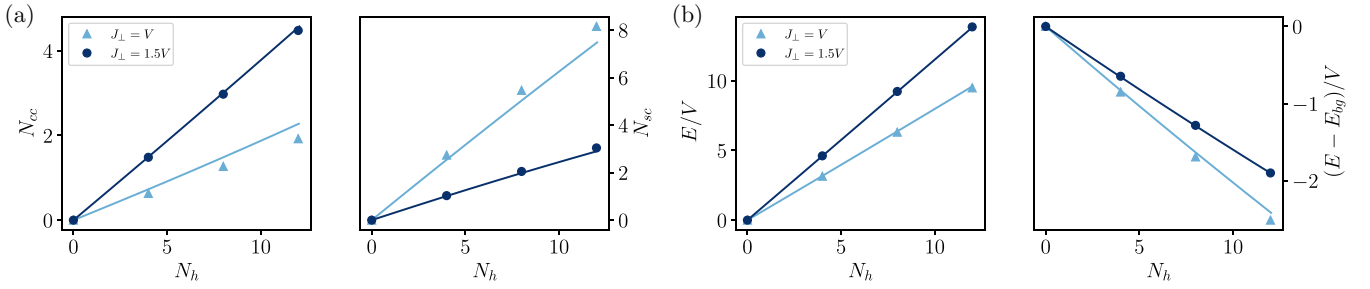


FIG. 4. Quasiparticle densities and ground state energy for the doped two-ladder system. (a) We compare the number of *sc* and *cc* pairs for a two-ladder system with  $L_x = 30$  and  $L_y = 2$  as the number of holes is tuned. We show the DMRG (markers) and mean-field (solid lines) for  $J_{\perp} = V$  and  $J_{\perp} = 1.5V$ , where  $t_{\parallel} = 0.1V$  is fixed. (b) The ground state energy  $E$  (left) of the microscopic model for a two-ladder system from DMRG (markers) is compared to the mean-field prediction for the effective Hamiltonian (solid lines). We also show the results for the ground state energies without considering the contribution from the background distortion  $E - E_{bg} = E - J_{\perp}N_{sc} - (V + J_{\perp})N_{cc}$  (right).

$E_{N_h} \approx 2(\min_k(E_k)) - 0 = 2\min_k(E_k)$ , which corresponds to the pairing gap obtained by diagonalizing the BCS mean-field Hamiltonian; see Supplemental Material [34]. As shown in Fig. 5, we find that as  $\frac{J_{\perp}}{V}$  increases, the binding energy  $E_B$  becomes larger, in agreement with the picture of tightly bound pairs of holes [26,28]. The values obtained from the mean-field calculations qualitatively follow the results from DMRG simulations. Another indication that the system undergoes a BCS-to-BEC crossover is obtained by comparing the binding energy  $E_B$  of the fermion pairs with the order parameter  $\Delta_k$  evaluated at  $k^*$  where the band gap is minimal  $\Delta_k^{\min} = \Delta_k(k^*)$ , where  $k^* = \arg \min(E_k)$ . This accounts for the phase coherence between the pairs: In the BCS region of extended pairs, the two quantities converge since pairs form and develop phase coherence at the same energy, whereas they are significantly different in the BEC regime, where fermions pair up with binding energy  $E_B$  but the condensation energy is lower [39,40]. This is a hallmark of the BCS-to-BEC crossover.

Furthermore, the mean-field description provides direct access to the order parameters characterizing the BEC and

BCS regimes. A key requirement for these order parameters is that they remain well-defined in the thermodynamic limit,  $L \rightarrow \infty$ . To this end, we define

$$\mathcal{O}_{\text{BEC}} = \sqrt{\frac{N_{cc}}{L^d}}, \quad (11)$$

$$\mathcal{O}_{\text{BCS}} = \frac{1}{L^d} \sum_k \frac{|\Delta_k|}{\sqrt{\Delta_k^2 + \xi_k^2}} \xrightarrow{L \rightarrow \infty} \frac{1}{(2\pi)^d} \times \int_{\text{BZ}} d^d k \frac{|\Delta_k|}{\sqrt{\Delta_k^2 + \xi_k^2}}, \quad (12)$$

which correspond to the BEC and BCS order parameters, respectively, for a  $d$ -dimensional system. The summation over the Brillouin zone (BZ) ensures that the order parameter is defined without resolving individual momentum states in  $k$ -space. In Fig. 6, we analyze a 2D bilayer system  $d = 2$ . This analysis confirms our picture of a BCS-to-BEC crossover around  $\frac{J_{\perp}}{V} \approx 1.4$ .

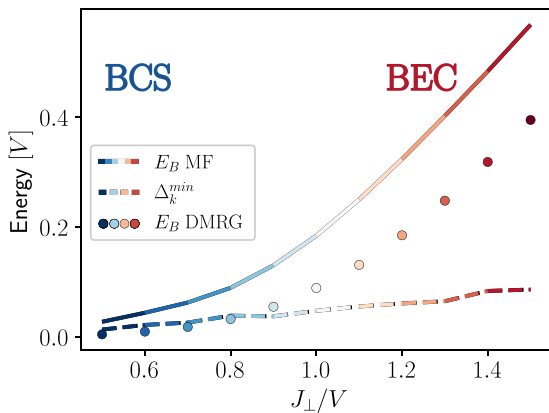


FIG. 5. The binding energies  $E_B$  computed for a 1D ladder system via DMRG (markers) is compared to mean-field theory (solid line) as  $J_{\perp}$  is tuned. Here, we also show the value of the order parameter  $\Delta_k$  at the minimum of  $E_k$ , i.e., where the band gap is minimal (dashed line). We consider a ladder system of size  $L = 30$  with fixed doping  $\delta = \frac{14}{30}$  and  $\frac{t_{\parallel}}{V} = 0.1$ .

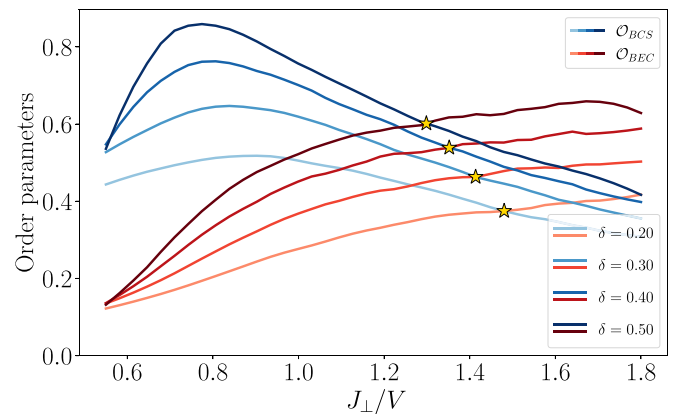


FIG. 6. We show the order parameters for the BEC and BCS regimes of the ansatz wave function in a 2D bilayer system, as defined in the main text. Here we consider a system of size  $L_x = L_y = 16$  for doping  $\delta = \{\frac{38}{256}, \frac{64}{256}, \frac{89}{256}, \frac{115}{256}\}$  at fixed  $t_{\parallel} = 0.1V$ . The stars mark the crossing point for each doping level.

#### IV. EXTENDED S-WAVE PAIRING IN 2D MIXD + V MODELS

In the previous section, we compared the mean-field predictions for different observables with the DMRG simulations of the microscopic model in 1D. This showed that the MixD + V ladder under consideration realizes a BCS-to-BEC crossover as  $\frac{J_{\perp}}{V}$  and  $\delta$  are tuned. The similarly good agreement in the quasi-2D ladder system in Fig. 4 indicates that our mean-field approach can be extended to true 2D bilayer systems, thereby granting access to the pairing gap without making any assumption on its symmetry. Indeed, the  $sc$ 's in the system pair up in singlets on opposite layers and are effectively described by the BCS wave function in Eq. (9), which is characterized by the parameter  $\Delta_k$ , defined in the Supplemental Material [34]. Figure 6 shows that the 2D crossover closely parallels the 1D case: As the interlayer AFM coupling  $J_{\perp}$  grows, extended  $sc$  pairs are replaced by tightly bound  $cc$  pairs, marking a BCS-BEC transition. Increasing the doping from 0.2 to 0.5 shifts this crossover to lower  $\frac{J_{\perp}}{V} \in (1.2, 1.5)$ , consistent with the quasiparticle densities in Fig. 3(a), which likewise show earlier  $cc$  dominance at higher doping. Although this is a smooth crossover rather than a sharp phase transition, its midpoint provides a useful indicator of the underlying shift in pairing character. Moreover, as shown in Fig. 2, the pairing function associated with the  $(sc)^2$  in a bilayer square lattice system features an extended  $s$ -wave symmetry, i.e., it presents a symmetric nontrivial momentum dependence with a clear nodal region and sign inversion.

This prediction is particularly intriguing in the light of the results from Ref. [11], where Cooper pairing with  $s_{\pm}$ -wave symmetry was found using functional renormalization group techniques. We note that recent two-orbital calculations for  $\text{La}_3\text{Ni}_2\text{O}_7$  show that the superconducting gap symmetry is highly sensitive to the  $\text{Ni-}e_g$  crystal-field splitting  $\Delta_{\text{CF}}$ : tuning  $\Delta_{\text{CF}}$  alters the relative strength of intra- and interlayer superexchange and can drive a transition from  $d_{xy}$  to  $s_{\pm}$  pairing [41]. The pairing gap that we obtain in our mean-field analysis has a simple structure and shows only two distinct areas in the Brillouin zone with different signs. We argue that this is due to the assumption of pointlike  $sc$ 's and  $cc$ 's which is valid in the tight-binding regime  $t_{\parallel} \ll V, J_{\perp}$ . However, additional features of the pairing gap are expected to appear when considering the internal structure of the constituents which becomes relevant for larger  $t_{\parallel}$ . Specifically, allowing recombination of  $sc$ 's and  $cc$ 's along the diagonal directions of the lattice, leads to the formation of a third region at the corners of the Brillouin zone; see Fig. 7. The diagonal recombination is implemented in the Hamiltonian of Eq. (3) by introducing the term

$$\hat{\mathcal{H}}_{\text{diag rec}}^{sc,cc} = -\epsilon \frac{t_{\parallel}}{\sqrt{2}} \sum_{i,j} \sum_{\mu,\sigma} (-1)^{\sigma} \hat{p}_f (\hat{f}_{i\mu\sigma}^{\dagger} \hat{f}_{j\bar{\mu}\bar{\sigma}}^{\dagger} \hat{b}_j + \text{H.c.}) \hat{p}_f, \quad (13)$$

where  $\epsilon$  tunes the strength of the interaction between the two channels along the  $i, j$  diagonal neighbors.

#### V. CONCLUSION

In conclusion, we have explored the physics of the MixD + V bilayer system and its implications for high- $T_c$  supercon-

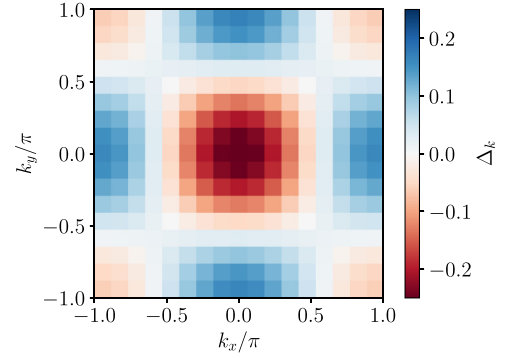


FIG. 7. The pairing gap  $\Delta_k$  is modified by the introduction of diagonal recombinations of  $sc$ 's and  $cc$ 's and an additional region with opposite sign appears at the corners of the Brillouin zone. Here we consider a 2D MixD + V model on a  $16 \times 16$  square lattice with  $\frac{t_{\parallel}}{V} = 0.1$ ,  $J_{\perp} = V$ ,  $\delta = \frac{104}{256}$  holes in the system, and with  $\epsilon = 1.5$ .

ductivity in the bilayer nickelate  $\text{La}_3\text{Ni}_2\text{O}_7$  (LNO). Previous work [20–23,25,28,30] identified two different regimes upon hole doping the effective low-energy model of these materials: on one side, the BCS region of spatially extended  $sc$  Cooper pairs, and on the other, the BEC region of tightly bound  $cc$ 's. Additionally, our numerical analysis indicates that in the BCS limit, pairing between  $sc$ 's arises from a Feshbach resonance, in analogy with atomic physics. However, a microscopic understanding of the intermediate regime was lacking. In this study, starting from the microscopic model, we derived an effective Hamiltonian in terms of the  $sc$ 's and  $cc$ 's, and proposed an ansatz ground state wave function to capture the essential physics of the charge carriers across the BCS-to-BEC crossover. The formulation of the mean-field theory allowed us to gain a microscopic understanding of the system by constructing a clear conceptual framework where the emergent constituents and their interactions could be investigated. By comparison with DMRG simulations in ladder systems, we have demonstrated the validity of the model and showed that it effectively describes the low energy physics of the system. Notably, the main result of this work is the prediction of a pairing gap with extended  $s$ -wave symmetry in the bilayer model, which characterizes the  $(sc)^2$  Cooper pairs. Our finding paves the way to explore even more complex scenarios by considering the internal structure of the charge carriers, which we propose will lead to additional features in the pairing gap, see Fig. 7. Lastly, we remark that the MixD + V bilayer system can be studied using ultracold atom experiments by a modification of the setup in Ref. [26], incorporating nearest-neighbor repulsion [25].

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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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