Editors' Suggestion

Type-II $t-J$ model and shared superexchange coupling from Hund's rule in superconducting $La_3Ni_2O_7$

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Recently, an 80 K superconductor was discovered in $La_3Ni_2O_7$ under high pressure. Density function theory calculations identify $d_{x^2-y^2}$, d_{z^2} as the active orbitals on the bilayer square lattice with a d^{8-x} configuration of Ni per site. Here, x is the hole doping level. One naive expectation is to describe this system in terms of a two-orbital t-J model. However, we emphasize the importance of Hund's coupling J_H and the $x=0$ limit should be viewed as a spin-one Mott insulator. Especially, the significant Hund's coupling shares the interlayer superexchange $J_\perp$ of the d_{z^2} orbital to the $d_{x^2-y^2}$ orbital, an effect that cannot be captured by conventional perturbation or mean-field approaches. This study first explores the limit where the d_{z^2} orbital is Mott localized, dealing with a one-orbital bilayer t-J model focused on the $d_{x^2-y^2}$ orbital. Notably, we find that strong interlayer pairing survives up to $x=0.5$ hole doping driven by the transmitted $J_\perp$, which explains the existence of a high Tc superconductor in the experiment at this doping level. Next, we uncover the more realistic situation where the d_{z^2} orbital is slightly hole-doped and cannot be simply integrated out. We take the $J_H\to+\infty$ limit and propose a type II t-J model with four *spin-half* singlon (d^7) states and three *spin-one* doublon (d^8) states. Employing a parton mean-field approach, we recover similar results as in the one-orbital t-J model, but now with the effect of the $J_\perp$ automatically generated.

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I. INTRODUCTION

Recently a superconductor with $T_c=80$K was found in $La_3Ni_2O_7$ under high pressure [1], following previous discoveries of superconductivity in nickelate $Nd_{1-x}Sr_xNiO_2$ [2] and also in $Nd_6Ni_5O_{12}$ [3] at ambient pressure. The discovery has triggered many experimental [4,5] and theoretical [4–15] studies. The average valence of Ni is in d^{8-x} with hole doping level, $x=0.5$ [1]. Density functional theory (DFT) calculations identify a bilayer square lattice structure with active $d_{x^2-y^2}$ and d_{z^2} orbitals, which we label as d_1 and d_2 in the following. The density (summed over spin) per site is estimated to be $n_1\approx 1-x=0.5$ and $n_2\approx 1$, so that the d_{z^2} orbital is close to Mott localization. Due to a large interlayer hybridization of the d_{z^2} orbital, we expect that it just forms a rung singlet when $n_2=1$. The d_{z^2} orbital has a small intralayer hopping, thus we do not expect a strong superconductivity from it. Then one may expect that superconductivity originates from the $d_{x^2-y^2}$ orbital. But the $d_{x^2-y^2}$ orbital is at hole doping level of 50%. According to the phase diagram of cuprates, it should be in the overdoped Fermi liquid phase. A major goal of this paper is to identify the minimal model to describe the nickelate superconductor and also find a mechanism for the material to superconductor at such a large hole doping.

One important ingredient we identify is Hund's coupling J_H between the d_{z^2} and the $d_{x^2-y^2}$ orbital. Due to the J_H coupling, the $x=0$ limit should be viewed as a spin-one Mott insulator formed by Ni^{2+}. The strong Hund's coupling J_H aligns the spin of the two orbitals at each site, then the large interlayer spin coupling $J_\perp$ of the d_{z^2} orbital is shared to the $d_{x^2-y^2}$ orbital. Therefore, when $n_2=1$, we can ignore the Mott localized d_{z^2} orbital (which is in a gapped rung-singlet phase) and phenomenologically consider a bilayer one-orbital t-J model for $d_{x^2-y^2}$ only. The model has a large interlayer spin coupling $J_\perp$ but without interlayer hopping $t_\perp$, a new situation not possible in the usual one-orbital Hubbard model. Through a slave-boson mean field calculation, we find that a large $J_\perp$ disfavors the familiar $d_{x^2-y^2}$ pairing at the $J_\perp=0$ limit and the system forms a strong s-wave superconductor with dominant interlayer pairing. But with a sufficiently large $J_\perp$, the pairing survives at $x=0.5$, which explains the superconductor at this hole doping level in the experiment. We note that a previous work has discussed quantitative renormalization effects of the Hund's coupling in flattening the bands [15], but the effect we identify here is qualitatively distinct and completely new. To our best knowledge the possibility of strong interlayer pairing for the $d_{x^2-y^2}$ orbital due to Hund's rule coupling to a rung-singlet phase of the d_{z^2} orbital has not been discussed previously.

The above treatment of 'integrating' out the d_{z^2} orbital is not very rigorous. Also, in the real system the d_{z^2} orbital may also be slightly hole doped. To be more precise and to enable the doping of the d_{z^2} orbital, we propose a bilayer type II t-J model to describe the low energy physics. The model is a generalization of a model proposed one of us before [16,17]. Basically we take the large J_H limit and restrict to a Hilbert space with four spin 1/2 singlon (d^7) states and three spin-one doublon (d^8) states. Inter-orbital J_H disappears in the model with the cost of non-trivial constraint. The type II t-J model can be understood to describe the low energy physics of doping a spin-one Mott insulator [18] with doped hole in a

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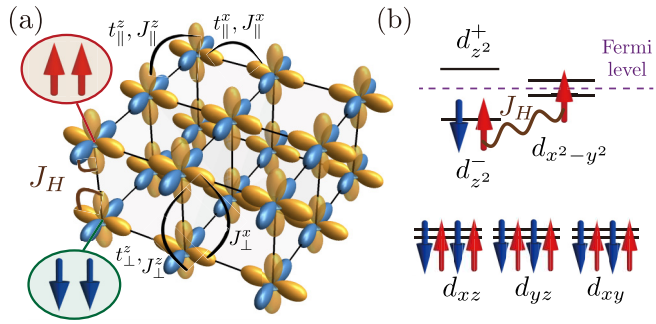

FIG. 1. (a) The schematics of the bilayer two-orbital model. The various t, J's are introduced for the hoppings and interactions of two orbitals on square lattices. Importantly, a strong ferromagnetic Hund coupling J_H transmits $J_\perp^z$ of the d_{z^2} orbital to the $d_{x^2-y^2}$ orbital, by enforcing a spin-triplet at each site (Inset). (b) The electronic configuration of two $Ni^{+2.5}$ states in one unit cell. The density per site with summing over spin is roughly $n_1 \simeq 1/2$ and $n_2 \simeq 1$.

spin 1/2 state. The model has two important parameters: the total hole doping level x and energy splitting Δ between the two orbitals to tune the relative doping of the two orbitals. In the large Δ limit, we have $n_2 = 1$ and d_{z^2} is Mott localized and forms a rung singlet. We propose a parton mean field theory to deal with the type II t-J model. In the simple large Δ limit, in the mean field level we reach a bilayer one-orbital t-J model for an emergent '$d_{x^2-y^2}$' orbital in the mean-field level. In this model, we can automatically get a large $J_\perp/t$ from our parton mean field theory, justifying our previous phenomenological treatment. From a direct mean field calculation of the type II t-J model, we find s-wave interlayer pairing at $x = 0.5$ similar to the one-orbital t-J model before.

II. BILAYER TWO-ORBITAL MODEL

We start from a two-orbital t-J model on a bilayer square lattice, Fig. 1(a), which has the following Hamiltonian:

$$H = H_K + J_\parallel^x \sum_l \sum_{\langle ij\rangle} \vec{S}_{i;l;1} \cdot \vec{S}_{i;l;1} + J_\perp^z \sum_i \vec{S}_{i;t;2} \cdot \vec{S}_{i;b;2} + U' \sum_i n_{i;1} n_{i;2} - 2J_H \sum_i \left(\vec{S}_{i;l;1} \cdot \vec{S}_{i;l;2} + \frac{1}{4} n_{i;1} n_{i;2} \right) \tag{1}$$

and

$$\begin{aligned} H_K = & -t_\parallel^x \sum_{l,\sigma} \sum_{\langle i,j\rangle} (P d_{i;l;1;\sigma}^\dagger d_{j;l;1;\sigma} P + \text{H.c.}) \\ & - t_\parallel^z \sum_{l,\sigma} \sum_{\langle i,j\rangle} (P d_{i;l;2;\sigma}^\dagger d_{j;l;2;\sigma} P + \text{H.c.}) \\ & - t_\parallel^{xz} \sum_{l,\sigma} \sum_{\langle ij\rangle} ((-1)^{s_{ij}} P d_{i;l;1;\sigma}^\dagger d_{j;l;2;\sigma} P + \text{H.c.}) \\ & - t_\perp^z \sum_i (P d_{i;t;2;\sigma}^\dagger d_{i;b;2;\sigma} P + \text{H.c.}) + \Delta \sum_i (n_{i;1} - n_{i;2}), \end{aligned}$$

where P is the projection operator to remove the double occupancy of each orbital. Here, $l = t, b$ labels the layer index, and $\sigma = \uparrow, \downarrow$ is for the spin index. We dub d_1, d_2 for the $d_{x^2-y^2}$ and d_{z^2} orbital, respectively. The hopping parameters are estimated $t_\parallel^x = 0.485, t_\parallel^z = 0.110, t_\parallel^{xz} = 0.239, t_\perp^z = 0.635$ by DFT [6]. $s_{ij} = 1$ for the x bond and $s_{ij} = -1$ for the y bond. For simplicity, we only keep intralayer $J_\parallel^x$ for the $d_{x^2-y^2}$ orbital and the interlayer $J_\perp^z$ for the d_{z^2} coupling. U' is inter-orbital repulsion and J_H is the Hund's coupling. $n_{i;a}$ is the density for orbital $a = 1, 2$. $\vec{S}_{i;l;a}$ is the spin operator for layer $l = t, b$ and orbital $a = 1, 2$. We also ignore the $n_i n_j$ term in the J coupling. In Fig. 1, we illustrate the system and the model. On average we have $n = 2 - x$ number of electrons (summed over spin) per site with $x \approx 0.5$ in the experiment. We have $n_1 \approx 0.5$ and $n_2 \approx 1$.

III. BILAYER ONE-ORBITAL T-J MODEL

We first consider the limit where the d_2 orbital is Mott localized with pinned $n_2 = 1$. In this limit, d_2 orbitals form a rung-singlet insulator due to large $J_\perp$ and may be integrated out and one can focus on an one-orbital t-J model with the d_1 orbital. However, we emphasize that the gapped d_2 degree of freedom still plays an important role due to the Hund's coupling. A large Hund's coupling enforces the two orbitals to form a spin-triplet at each site. Within the restricted Hilbert space, the spins of the two orbitals align and the interlayer spin-spin coupling $J_\perp^z$ also induces anti-ferromagnetic coupling of the d_1 orbital [see the inset of Fig. 1(a)]. Basically only the orbital symmetric part, $J_\perp^x = J_\perp^z$, can persist in the restricted Hilbert space. Consequently, we should consider a significant interlayer $J_\perp$ also for the $d_{x^2-y^2}$ orbital, though there is no interlayer hopping.

Motivated by the above considerations, we now consider an effective one-orbital t-J model for the $d_{x^2-y^2}$ orbital,

$$\begin{aligned} H_{\text{eff}} = & -t_\parallel^x \sum_{l,\sigma} \sum_{\langle i,j\rangle} P(d_{i;1;l,\sigma}^\dagger d_{j;1;l;\sigma}) P + \text{H.c.} \\ & + J_\parallel^x \sum_l \sum_{\langle i,j\rangle} \vec{S}_{i;l;1} \cdot \vec{S}_{j;l;1} + J_\perp^z \sum_i \vec{S}_{i;t;1} \cdot \vec{S}_{i;b;1}. \end{aligned} \tag{2}$$

Hereafter, shorthand notations $t = t_\parallel^x, J_\parallel = J_\parallel^x$, and $J_\perp = J_\perp^z$ are used, unless otherwise stated. Note that the model above is quite unconventional in the sense that we have a large $J_\perp$ but no interlayer hopping $t_\perp$, compared to other existing models [19]. This is impossible in the standard t-J model usually with $J < t$. We note a similar model (dubbed as mixed dimensional t-J model) has been proposed in the cold atom context but only out of equilibrium [20,21].

We then employ the standard U(1) slave-boson mean-field theory [22] and represent the electronic operator as, $d_{i;l;1;\sigma}^\dagger = f_{i;l;\sigma}^\dagger b_{i;l}$ with the constraint $n_{i;l;f} + n_{i;l;b} = 1$ [see the Appendices for details]. In the mean-field level, we decouple the following order parameters from the J terms: the hopping terms $\chi_{\parallel;ij,\sigma}^l = 2\langle f_{i;l;\sigma}^\dagger f_{j;l;\sigma}\rangle$, $\chi_{\perp;i;\sigma} = 2\langle f_{i;t;\sigma}^\dagger f_{i;b;\sigma}\rangle$ and the pairing terms $\Delta_{\parallel;ij}^l = 2s^{ij}\langle f_{i;l;\uparrow} f_{j;l;\downarrow}\rangle$, $\Delta_{\perp;i} = 2\langle f_{i;t;\uparrow} f_{i;b,\downarrow}\rangle$. We obtain these order parameters from self-consistent calculations. We fix $t_\parallel = 1$ and $J_\parallel = 1/2$ and vary the $J_\perp$ and the doping x in the range $0 \leqslant x \leqslant 1/2$.

Here, we summarize our numerical results. In the limit of small $J_\perp$, the model reproduces the well-known behaviors of the single-layer t-J model, with the famous $d_{x^2-y^2}$ pairing within each layer. As the strength of $J_\perp$ is gradually increased, there is a first-order transition after which we find s-wave

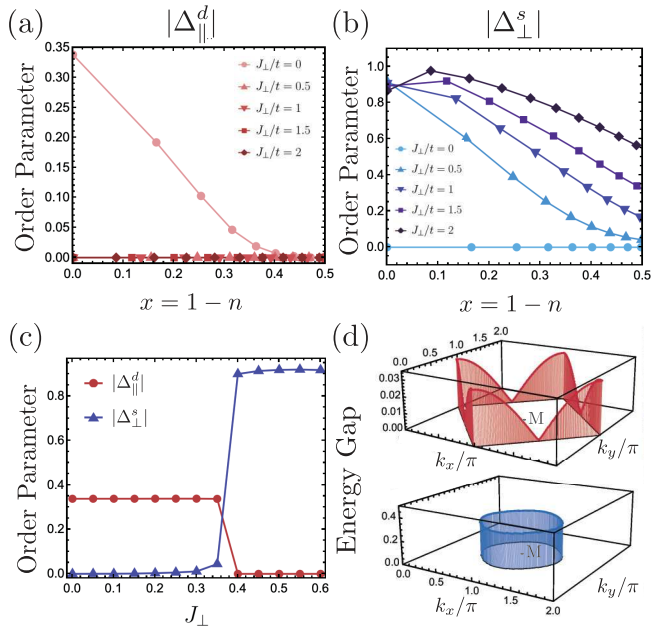

FIG. 2. [(a), (b)] Zero temperature mean-field solutions of one-orbital t-J model. We plot the filling x dependence of (a) intralayer d-wave pairing, (b) interlayer s-wave pairing within the slave-boson framework are shown at $t^x_\parallel = 1$, $J^x_\parallel = 1/2$. (c) $J_\perp$ dependence of pairing order parameter at $x = 0$. The inclusion of $J^z_\perp$ induces the first-order phase transition from d-wave pairing, $\Delta^d_\parallel$, to s-wave pairing, $\Delta^s_\perp$. (d) The energy gap of the two distinct superconducting states at the Fermi surface. Two specific cases of $J^z_\perp/t^x_\parallel = 0, x = 0$ (top) and $J^z_\perp/t^x_\parallel = 2, x = 1/2$ (bottom) are chosen for a illustration. The normal Fermi surface, centered at the $\mathrm{M} = (\pi, \pi)$ point, is completely gapped with an s-wave pairing (bottom), while there are four point nodes with a d-wave pairing (top).

pairing with dominated interlayer pairing, as illustrated in Figs. 2(a) and 2(b). In Fig. 2(c), we find a first-order transition from the d-wave to s-wave pairing with dominated interlayer pairing. With a large enough $J_\perp$ (for example, $J_\perp/t > 0.5$), the value of $|\Delta_\perp|$ remains survives to the large hole doping regime with $x \simeq 0.5$.

We note that the normal Fermi surfaces are completely gapped in the s-wave pairing phase, while there are nodes in the d-wave pairing, as depicted in Fig. 2(d). $J_\perp/t > 0.5$ is quite reasonable given that $J_\perp$ origins from the superexchange of the d_2 orbital which has a large interlayer coupling. Thus we expect an s-wave interlayer paired superconductor in the experimental regime even with a 50% hole doping. We emphasize that it is important to have large $J_\perp$ but with the interlayer hopping $t_\perp = 0$. For example, one can imagine a conventional bilayer t-J model for the d_{z^2} orbital with $t_\perp > J_\perp$. In Fig. 3, we show that a large $t_\perp$ term suppresses the pairing because the hopping disfavors interlayer spin-singlet Cooper pair. Therefore the unusual model we consider here for the $d_{x^2-y^2}$ orbital host has stronger pairing than the usual t-J model.

IV. TYPE-II T-J MODEL

The importance of Hund's coupling in sharing the superexchange J has been demonstrated in the simple case of $n_2 = 1$ per site. In this limit, the d_2 orbital is orbital-selective Mott

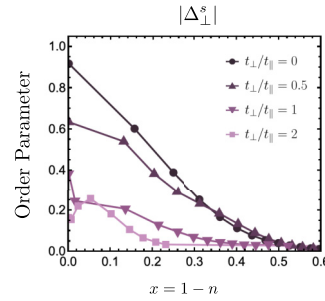

FIG. 3. Mean-field order parameters of the one-orbital model. Inter-layer hopping $t_\perp$ dependence of the interlayer pairing at $J_\perp = 1/2$. The inclusion of larger inter-layer hopping $t_\perp$ suppressed the inter-layer pairing order parameter $\Delta_\perp$.

localized and forms a rung-singlet. Then we just ignore d_2 and deal with a one-orbital model and take the transmission of $J_\perp$ by hand. However, this approach is not very rigorous and needs a justification. Moreover, in the real system, the d_2 orbital is likely to be slightly hole doped with $n_2 < 1$. Then the d_2 orbital should be kept in the low energy model. In this case, we need to deal with the full two-orbital model in Eq. (1). However, U' and J_H are large and cannot be treated in perturbation or mean field level. Especially, there is no good way to capture the effect of sharing the J terms between the two orbitals from the Hund's coupling. Apparently, a new model and a new method is called for to describe the realistic regimes with two active orbitals and a strong Hund's coupling.

To address this challenging problem, we take a non-perturbative approach. We first take U', J_H to be large and project to a restricted Hilbert space. This leads to a generalization of the type II t-J model proposed by one of us in Ref. [16]. We only keep four singlon (d^7) states and three spin-triplet doublon (d^8) states. First, at each site i, the four singlon states can be labeled as, $|a\sigma\rangle = d^\dagger_{a;\sigma}|G\rangle$ where $|G\rangle$ is defined as a vacuum states where all t_{2g} orbitals are fully filled with $a = 1, 2$ and $\sigma = \uparrow, \downarrow$. Meanwhile, the three spin-triplet doublon states are written as $|-1\rangle = d^\dagger_{1\downarrow} d^\dagger_{2\downarrow}|G\rangle$, $|0\rangle = \frac{1}{\sqrt{2}}(d^\dagger_{1\uparrow} d^\dagger_{2\downarrow} + d^\dagger_{1\downarrow} d^\dagger_{2\uparrow})|G\rangle$, and $|1\rangle = d^\dagger_{1\uparrow} d^\dagger_{2\uparrow}|G\rangle$. Here, we ignore the site index i for simplicity. The spin-singlet doubly occupied states are penalized by a large J_H and are removed from the Hilbert space.

Now, we project the electron operator inside this $4 + 3 = 7$ dimensional Hilbert space:

$$
\begin{aligned}
d_{i;l;1\uparrow} &= \prod_{j<i}(-1)^{n_j}\left(|2\uparrow\rangle_{il}\langle 1|_{il} + \frac{1}{\sqrt{2}}|2\downarrow\rangle_{il}\langle 0|_{il}\right),\\
d_{i;l;1\downarrow} &= \prod_{j<i}(-1)^{n_j}\left(|2\downarrow\rangle_{il}\langle -1|_{il} + \frac{1}{\sqrt{2}}|2\uparrow\rangle_{il}\langle 0|_{il}\right),\\
d_{i;l;2\uparrow} &= -\prod_{j<i}(-1)^{n_j}\left(|1\uparrow\rangle_{il}\langle 1|_{i\,l} + \frac{1}{\sqrt{2}}|1\downarrow\rangle_{il}\langle 0|_{il}\right),\\
d_{i;l;2\downarrow} &= -\prod_{j<i}(-1)^{n_j}\left(|1\downarrow\rangle_{il}\langle -1|_{il} + \frac{1}{\sqrt{2}}|1\uparrow\rangle_{il}\langle 0|_{il}\right), \quad (3)
\end{aligned}
$$

where $\prod_{j<i}(-1)^{n_j}$ is the Jordan-Wigner string. The spin operators for the *spin-1/2* singlon state are $\vec{s}_{i;a} = \frac{1}{2}\sum_{\sigma\sigma'} |a\sigma\rangle_i \vec{\sigma}_{\sigma\sigma'} \langle a\sigma'|_i$ with $\vec{\sigma}$ as the Pauli matrices. the spin operators for the *spin-one* doublon states are written as $\vec{S}_i = \sum_{\alpha,\beta=-1,0,1} \vec{T}_{\alpha\beta}|\alpha\rangle_i\langle\beta|_i$. Here, we have $T_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ and $T_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$ in the $|1\rangle, |0\rangle, |-1\rangle$ basis.

The type II t-J model Hamiltonian is

$$\begin{aligned} H = H_K &+ J_\parallel^x \sum_l \sum_{\langle ij\rangle} \vec{s}_{i;l;1} \cdot \vec{s}_{j;l;1} + J_\perp^z \sum_i \vec{s}_{i;t;2} \cdot \vec{s}_{i;b;2} \\ &+ J_{sd}^\parallel \sum_l \sum_{\langle ij\rangle} (\vec{s}_{i;l;1} \cdot \vec{S}_{j;l} + \vec{S}_{i;l} \cdot \vec{s}_{j;l;1}) \\ &+ J_{sd}^\perp \sum_i (\vec{s}_{i;t;2} \cdot \vec{S}_{i;b} + \vec{S}_{i;t} \cdot \vec{s}_{i;b;2}) \\ &+ J_{dd}^\parallel \sum_l \sum_{\langle ij\rangle} \vec{S}_{i;l} \cdot \vec{S}_{j;l} + J_{dd}^\perp \sum_i \vec{S}_{i;t} \cdot \vec{S}_{i;b}, \end{aligned} \tag{4}$$

where H_K is the same as in Eq. (1), except that the above projected electron operators are in the $4+3=7$ Hilbert space as defined above. We have $J_{sd}^\parallel = \frac{1}{2}J_\parallel^x, J_{sd}^\perp = \frac{1}{2}J_\perp^z, J_{dd}^\parallel = \frac{1}{4}J_\parallel^x$, and $J_{dd}^\perp = \frac{1}{4}J_\perp^z$. We are interested in the filling of $n_T = n_1 + n_2 = 1 + n = 2 - x$. If the number of sites is N_S, there are $(1-x)N_s$ number of doublon states and xN_s number of singlon states. The energy splitting Δ in H_K tunes the relative density of the two orbitals. In particular, if Δ is large and positive, we only need to keep two singlon states corresponding to the d_2 orbital.

V. PARTON MEAN-FIELD THEORY

We employ the three-fermion parton construction [16] to deal with the type II t-J model. The four singlon states are constructed as $|a\sigma\rangle_i = f_{i;a\sigma}^\dagger|0\rangle$, while the three $S=1$ doublons are created by $|-1\rangle_i = \psi_{i;1\downarrow}^\dagger\psi_{i;2\downarrow}^\dagger|0\rangle$, $|0\rangle_i = \frac{1}{\sqrt{2}}(\psi_{i;1\uparrow}^\dagger\psi_{i;2\downarrow}^\dagger - \psi_{i;2\uparrow}^\dagger\psi_{i;1\downarrow}^\dagger)|0\rangle$, and $|1\rangle = \psi_{i;1\uparrow}^\dagger\psi_{i;2\uparrow}^\dagger|0\rangle$. We need to impose a local constraint at each site i: $n_{i;f} + n_{i;\psi_1} = 1$, $n_{i;\psi_1} = n_{i;\psi_2}$ with $n_{i;f} = \sum_{a\sigma} f_{i;a\sigma}^\dagger f_{i;a\sigma}$ and $n_{i;\psi_a} = \sum_\sigma \psi_{i;a\sigma}^\dagger\psi_{i;a\sigma}$. On average, we have $n_f = x$ and $n_{\psi_1} = n_{\psi_2} = 1 - x$ with the convention $n_1 + n_2 = 2 - x$. We introduce the notation $\Psi_{i;\sigma} = (\psi_{i;1\sigma}, \psi_{i;2\sigma})^T$, then there is another constraint: $\Psi_i^\dagger\vec{\tau}\Psi_i = 0$, where $\vec{\tau}$ is the Pauli matrix in the color space. This constraint enforces the two colors $a = 1, 2$ forms singlet, thus the spin is in a triplet due to fermion statistics [16]. This constraint gives a SU(2) gauge symmetry: $\Psi_i \to U_i\psi_i$, where $U_i \in SU(2)$ acting in the color space, rotating ψ_1 to ψ_2.

Within the parton construction, the projected electron operator is represented as, $d_{i;a\sigma} = \epsilon_{ab} f_{i;b\sigma}^\dagger \psi_{i;2\sigma}\psi_{i;1\sigma} + \frac{1}{2}\epsilon_{ab} f_{i;b\bar{\sigma}}^\dagger(\psi_{i;2\downarrow}\psi_{i;1\uparrow} + \psi_{i;2\uparrow}\psi_{i;1\downarrow})$. Here, ϵ_{ab} is the antisymmetric tensor with $\epsilon_{12} = 1$ and $\bar{\sigma}$ denotes the opposite spin of σ. The singlon and doublon spin operators are now represented as $\vec{s}_{i;a} = \frac{1}{2}\sum_{\sigma,\sigma'} f_{i;a\sigma}^\dagger \vec{\sigma}_{\sigma\sigma'} f_{i;a\sigma'}$ and $\vec{S}_i = \frac{1}{2}\sum_a \sum_{\sigma\sigma'} \psi_{i;a\sigma}^\dagger \vec{\sigma}_{\sigma\sigma'} \psi_{i;a\sigma'}$.

Substituting all the above expressions, one can decouple the type II t-J model in Eq. (4) and perform the self-consistent mean-field calculation. We provide all details in the Appendices. In principle, one can have a phase diagram from tuning Δ and x. For simplicity, we here consider the large positive Δ limit, so that n_2 is pinned to be 1, safely ignoring f_1 and keeping only the two singlon states occupied by $f_{2\sigma}$. This corresponds to orbital selective Mott localization of the d_{z^2} orbital and now $d_{i;2\sigma} = 0$ without the f_1 operator. One important mean field decoupling is an on-site term, $\langle\psi_{i;l;a\sigma}^\dagger f_{i;l;2\sigma}\rangle = \frac{3}{4}\Phi_a$ for each spin σ component. Due to the SU(2) gauge symmetry, we can always fix the gauge to choose $\Phi_2 \neq 0$ while $\Phi_1 = 0$. Then $\langle\psi_{i;l;2\sigma}^\dagger f_{i;l;2\sigma}\rangle = 3\Phi_2/4 \neq 0$ and we have $d_{i;l;1\sigma} \sim \frac{3}{4}\Phi_2^\dagger\psi_{i;l;1\sigma}$. Now $\psi_{i;l;1\sigma}$ can be identified as the electron operator of the $d_{x^2-y^2}$ orbital with density $n_{\psi_1} = 1 - x$, while f_2 and ψ_2 hybridize and form the same band with the total density $n_{f_2} + n_{\psi_2} = 1$ per site. They just represent the localized spin moments of the d_{z^2} orbital and form a rung singlet in the bilayer model due to the large $J_\perp^z$ term.

In terms of the emergent '$d_{x^2-y^2}$' orbital ψ_1, an effective model can be derived from Eq. (4) by substituting $d_{i;l_1\sigma} \sim \frac{3}{4}\Phi_2^\dagger\psi_{i;l;1\sigma}$:

$$\begin{aligned} H_{\psi_1} = \sum_l \sum_{\langle ij\rangle} \Big[&- \frac{9}{16}|\Phi_2|^2 t_\parallel^x \psi_{i;l;1\sigma}^\dagger \psi_{i;l;1\sigma} \\ &+ J_{dd}^\parallel \vec{S}_{i;l;\psi_1} \cdot \vec{S}_{j;l;\psi_1} \Big] + J_{dd}^\perp \sum_i \vec{S}_{i;t;\psi_1} \cdot \vec{S}_{i;b;\psi_1}, \end{aligned} \tag{5}$$

where $\vec{S}_{i;l;\psi_1} = \frac{1}{2}\psi_{i;l;1\sigma}^\dagger \vec{\sigma}_{\sigma\sigma'}\psi_{i;l;1\sigma'}$ is the spin operator of ψ_1. The effective spin-spin coupling for this emergent ψ_1 orbital originates from the J_{dd} coupling of the spin-one moments. As a result, the superexchange of both d_{z^2} and $d_{x^2-y^2}$ orbitals contribute to the J coupling of this effective model. We have a large $J_{dd}^\perp = \frac{1}{4}J_\perp^z$ and large $J_{dd}^\parallel = \frac{1}{4}J_\parallel^x$ for this emergent $\psi_1 \sim d_1$ orbital, even though there is no interlayer hopping. We also note an interesting effect of reducing the hopping by a factor of $|\Phi_2|^2$ ($|\Phi_2| < 0.5$ from our calculation as in Fig. 5(c) in Appendix B. We perform a fully self-consistent mean field calculation involving all f_2, ψ_1, ψ_2 orbitals. We confirm that f_2, ψ_2 just form a band insulator in agreement with a rung-singlet phase, while the ψ_1 orbital is at density $n_1 = 1 - x$ and gets intralayer and interlayer pairing terms as shown in Figs. 4(a) and 4(b). Note that we still use t, $J_\parallel$, and $J_\perp$ as abbreviations of $t_\parallel^x$, $J_\parallel^x$, and $J_\perp^z$, and set $t = 1$, $J_\parallel = 1/2$. Varying $J_\perp$, we again find a first-order transition from the familiar d-wave to s-wave pairing with dominated interlayer pairing [see Fig. 5(d)]. If we take a large $J_\perp$ such as $J_\perp/t = 1$, the s-wave pairing is still large at $x = 0.5$. Overall, the results are qualitatively the same as the previous bilayer one-orbital t-J model [see Figs. 2(a) and 2(b)], justifying our previous treatment. However, now we achieve these results from a more precise approach of a microscopic model. The sharing of the superexchange of one orbital to the other orbital is automatically taken care of in our model and parton framework.

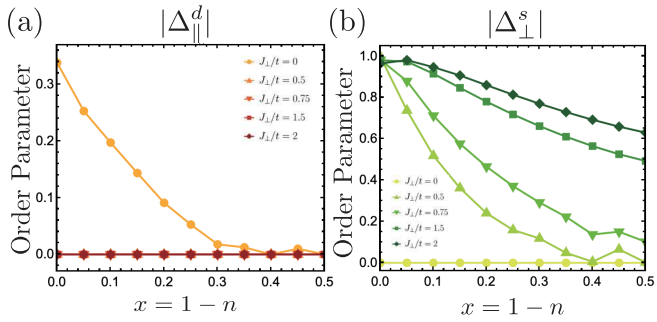

FIG. 4. [(a), (b)] Zero temperature mean-field solutions of type II t-J model in the large Δ limit. We plot the filling x dependence of (a) intralayer pairing, (b) interlayer pairing of the emergent '$d_{x^2-y^2}$' orbital at $t_{\parallel}^{x} = 1$, $J_{\parallel}^{x} = 1/2$. Comparing Figs. 2(a) and 2(b) here, we notice that the one-orbital t-J model shows similar behaviors as the more rigorous type II t-J model in the large Δ limit with the d_{z^2} Mott localized.

VI. DISCUSSION

The calculation in Fig. 2 is limited to the large Δ regime with the orbital d_{z^2} in a Mott localized state (forming a rung singlet). In the realistic system, we may have a smaller Δ and the d_{z^2} orbital may likely be slightly doped and also participate in the pairing. This will induce some quantitative effects: (1) d_{z^2} orbital also contributes to superconductivity; (2) The effective hole doping level of the $d_{x^2-y^2}$ can get reduced even though the total hole doping level is fixed; (3) The inter-orbital hopping may further transmit the pairing of one orbital to the other orbital. We note that a two-orbital t-J model has been proposed and studied for $La_3Ni_2O_7$ (for example, see Ref. [6]), but the previous works all ignore the important effect of sharing the superexchange J coupling between the two orbitals by the large Hund's coupling. We have demonstrated that this effect is crucial in the large Δ limit, so obviously it should not be ignored in the smaller Δ regime. With both orbitals active, we also cannot derive a one-orbital model simply by integrating the d_{z^2} orbital. In this regime, we believe the type II t-J model we propose here is the minimal model to capture all essential ingredients. A phase diagram of (Δ, x) can be obtained by extending our parton mean-field theory with f_1 orbital included, which we leave to future work.

We also emphasize the difference between our type II t-J model in Eq. (4) and the simplified one-orbital $t - J_{\parallel} - J_{\perp}$ model in Eq. (2). We here uncover the one-orbital model simply to demonstrate the essence of our mechanism of interlayer pairing. However, we emphasize here that Eq. (2) is not appropriate for nickelate at least quantitatively even if the d_{z^2} is Mott localized. Starting from the full model in Eq. (1), one can reach Eq. (2) by integrating the d_{z^2} orbital in the $J_H \ll J_{\perp}^{z}$ limit and get $J_{\perp} \sim \frac{J_H^2}{J_{\perp}^{z}}$. But we believe nickelate is in the $J_H \gg J_{\perp}^{z}$ limit because Hund's coupling J_H is part of the Coulomb interaction and should be large. Then the perturbative treatment obviously breaks down and we do not see any controlled way to reach the one-orbital t-J model in Eq. (2) from Eq. (1) in the large J_H regime. In the large J_H limit, the appropriate approach is to take the large J_H expansion instead, which leads to our type II t-J model in Eq. (4) in the leading order. In the type II t-J model, the localized spin moment from d_{z^2} orbital becomes also dynamical due to the coupling to the holes in the $d_{x^2-y^2}$ orbital. One possible effect is the polaron formation between the hole and the localized spin moment, as has already been demonstrated in a previous study of a one-dimensional type II t-J model [18]. Such polaron effect is completely ignored in the one-orbital t-J model. We believe the type II t-J model is the minimal model to capture all of the essential physics in the nickelate $La_3Ni_2O_7$.

VII. CONCLUSION

In summary, we propose and study a bilayer type II t-J model for the superconducting $La_3Ni_2O_7$ under high pressure. We emphasize the important role of the Hund's coupling between the $d_{x^2-y^2}$ and the d_{z^2} orbital, which enforces the d^8 state to be a spin-triplet. Due to the Hund's rule, the superexchange of one orbital can be shared to the other orbital. We propose a parton mean field treatment of the type II t-J model. In the limit that the d_{z^2} is Mott localized and forms a rung singlet, we reach a bilayer one-orbital t-J model without interlayer hopping, but with enhanced interlayer antiferromagnetic spin-spin coupling $J_{\perp}$ over intralayer hopping t. Mean field theory then predicts an s-wave interlayer paired superconductor even at hole doping 50%, in agreement with the experiment. In the future, one natural extension is to tune the orbital splitting Δ in our type II t-J model to make the d_{z^2} orbital also slightly hole doped.

Note added. When finalizing the manuscript, we became aware of a preprint [23] which also studied a bilayer one-orbital t-J model with strong interlayer $J_{\perp}$, which is the same as Eq. (2) of our paper. However, in our opinion, the correct model in the large J_H limit is the type II t-J model in Eq. (4) of our paper. These two models are different even when d_{z^2} is Mott localized, see our recent paper [24] for comparisons in numerical simulations of these two models.

ACKNOWLEDGMENT

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APPENDIX A: ONE-ORBITAL T-J MODEL AND SLAVE-BOSON THEORY

We start from the one-orbital Hamiltonian,

$$H = -t_{\parallel}^{x} \sum_{l,\sigma} \sum_{\langle i,j \rangle} P\left(d_{i;1;l,\sigma}^{\dagger} d_{1;l;\sigma}\right) P + \text{H.c.} + J_{\parallel}^{x} \sum_{l} \sum_{\langle i,j \rangle} \vec{S}_{i;l;1} \cdot \vec{S}_{i;l;1} + J_{\perp}^{z} \sum_{i} \vec{S}_{i;t;1} \cdot \vec{S}_{i;b;1}, \quad \text{(A1)}$$

and perform the mean field theory employing the slave boson representation, $d_{i;l,1,\sigma}^{\dagger} = f_{i;l;\sigma}^{\dagger} b_{i;l}$. Assuming $\langle b_i \rangle = \sqrt{x}$, after the mean-field decoupling, the mean-field Hamiltonian

is given by

$$\begin{aligned} H_{SB}^{MF} =& -t_{\parallel}\sum_{l,\sigma,\langle i,j\rangle}(f^{\dagger}_{i;l;\sigma}f_{j;l;\sigma}+\text{H.c.}) \\ & -t_{\perp}\sum_{\sigma,i}(f^{\dagger}_{i;t;\sigma}f_{i;b;\sigma}+\text{H.c.}) \\ & +D_{\parallel}\sum_{l,\langle i,j\rangle}(s_{ij}(f^{\dagger}_{i;l;1;\uparrow}f^{\dagger}_{j;l;1;\downarrow}-f^{\dagger}_{i;l;1;\downarrow}f^{\dagger}_{j;l;1;\uparrow})+\text{H.c.}) \\ & +D_{\perp}\sum_{i}(f^{\dagger}_{i;t;\uparrow}f^{\dagger}_{i;b;\downarrow}-f^{\dagger}_{i;t;\downarrow}f^{\dagger}_{i;b;\uparrow}+\text{H.c.}) \end{aligned} \tag{A2}$$

with the coefficients

$$t_{\parallel}=xt^{x}_{\parallel}+\tfrac{3}{8}J^{x}_{\parallel}\chi_{\parallel},\quad t_{\perp}=\tfrac{3}{8}J^{z}_{\perp}\chi_{\perp},$$
$$D^{\parallel}=\tfrac{3}{8}J^{x}_{\parallel}\Delta^{d}_{\parallel},\quad D^{\perp}=\tfrac{3}{8}J^{z}_{\perp}\Delta^{s}_{\perp}.$$

There are four mean field order parameters:

$$\chi_{\parallel}=\sum_{\sigma}\langle f^{\dagger}_{j;l;\sigma}f_{i;l;\sigma}\rangle,\quad \chi_{\perp}=\sum_{\sigma}\langle f^{\dagger}_{i;t;\sigma}f_{i;b;\sigma}\rangle, \tag{A3}$$

$$\begin{aligned} \Delta_{\parallel}&=\langle s^{ij}(f_{i;l;\uparrow}f_{j;l;\downarrow}-f_{i;l;\downarrow}f_{j;l;\uparrow})\rangle, \\ \Delta_{\perp}&=\langle f_{i;t;\uparrow}f_{j;b;\downarrow}-f_{i;t;\downarrow}f_{j;b;\uparrow}\rangle. \end{aligned} \tag{A4}$$

Moreover, the chemical potential should be fixed for conserving the particle number, $n=\sum_{k,l}\langle f^{\dagger}_{k;l;\sigma}f_{k;l;\sigma}\rangle=1-x$.

APPENDIX B: TYPE-II T-J MODEL AND THREE-FERMION PARTON THEORY

We start from the type II t-J model introduced in Eq. (4). Considering the large Δ limit, the singlon is formed by only d_2 orbital, thus the Hilbert space is restricted into $P_0=P-|1,\uparrow\rangle\langle 1,\uparrow|-|1,\downarrow\rangle\langle 1,\downarrow|$. In this Hilbert space, electron operators of d_2 orbital itself become zero, thus the kinetic Hamiltonian can be expressed in terms of d_1 orbital,

$$\begin{aligned} H =& -t^{x}_{\parallel}\sum_{l,\sigma,\langle i,j\rangle}(P_0 d^{\dagger}_{i;l;1;\sigma}d_{j;l;1;\sigma}P_0+\text{H.c.}) \\ & +J^{x}_{\parallel}\sum_{l,\langle i,j\rangle}\vec{s}_{i;l;1}\cdot\vec{s}_{j;l;1}+J^{dd}_{\parallel}\sum_{l,\langle i,j\rangle}\vec{S}_{i;l}\cdot\vec{S}_{j;l}+J^{sd}_{\parallel}\sum_{l,\langle i,j\rangle}(\vec{s}_{i;l;1}\cdot\vec{S}_{j;l}+\cdot\vec{S}_{i;l}\cdot\vec{s}_{j;l;1}) \\ & +J^{z}_{\perp}\sum_{i}\vec{s}_{i;t;2}\cdot\vec{s}_{i;b;2}+J^{dd}_{\perp}\sum_{i}\vec{S}_{i;t}\cdot\vec{S}_{i;b}+J^{sd}_{\perp}\sum_{i}(\vec{s}_{i;t;2}\cdot\vec{S}_{i;b}+\vec{S}_{i;t}\cdot\vec{s}_{i;b;2}). \end{aligned} \tag{B1}$$

Here, we use the following three-fermion decomposition:

$$d^{\dagger}_{i;l;1;\sigma}=(\psi^{\dagger}_{i;l;1;\sigma}\psi^{\dagger}_{i;l;2;\sigma})f_{i;l;2;\sigma}+\tfrac{1}{2}(\psi^{\dagger}_{i;l;1\uparrow}\psi^{\dagger}_{i;2;l;\downarrow}+\psi^{\dagger}_{i;1;l;\downarrow}\psi^{\dagger}_{i;2;l;\uparrow})f_{i;l;2;\bar{\sigma}}, \tag{B2}$$

$$d_{j;l;1;\sigma}=f^{\dagger}_{j;l;2;\sigma}(\psi_{j;l;2;\sigma}\psi_{j;l;1;\sigma})+\tfrac{1}{2}f^{\dagger}_{j;l;2;\bar{\sigma}}(\psi_{j;l;2;\downarrow}\psi_{j;l;1;\uparrow}+\psi_{j;l;2;\uparrow}\psi_{j;l;1;\downarrow}). \tag{B3}$$

Employing the standard decoupling principle, the mean-field Hamiltonian is given by

$$\begin{aligned} H^{MF}_{TF} =& -t_{f;2}\sum_{l,\sigma,\langle i,j\rangle}(f^{\dagger}_{i;l;2;\sigma}f_{j;l;2;\sigma}+\text{H.c.})-\sum_{a,c=1,2}t_{\psi;ac}\sum_{l,\sigma,\langle i,j\rangle}(\psi^{\dagger}_{i;l;a;\sigma}\psi_{j;l;c;\sigma}+\text{H.c.}) \\ & -\sum_{a=1,2}C^{0}_{a}\sum_{l,\sigma,i}(f^{\dagger}_{i;l;2;\sigma}\psi_{i;l;a;\sigma}+\psi^{\dagger}_{i;l;a;\sigma}f_{i;l;2;\sigma}+\text{H.c.})-t^{\perp}_{f}\sum_{\sigma,i}(f^{\dagger}_{i;t;2;\sigma}f_{i;b;2;\sigma}+\text{H.c.}) \\ & -\sum_{a,c=1,2}t^{\perp}_{\psi;ac}\sum_{\sigma,i}(\psi^{\dagger}_{i;t;a;\sigma}\psi_{i;b;c;\sigma}+\text{H.c.})-\sum_{a=1,2}C^{\perp}_{a}\sum_{\sigma,i}(f^{\dagger}_{i;t;2;\sigma}\psi_{i;b;a;\sigma}+\psi^{\dagger}_{i;t;a;\sigma}f_{i;b;2;\sigma}+\text{H.c.}) \\ & +D_{\psi;1}\sum_{l,\langle i,j\rangle}(s_{ij}(\psi^{\dagger}_{i;l;1;\uparrow}\psi^{\dagger}_{j;l;1;\downarrow}-\psi^{\dagger}_{i;l;1;\downarrow}\psi^{\dagger}_{j;l;1;\uparrow})+\text{H.c.})+D^{\perp}_{\psi;1}\sum_{i}(\psi^{\dagger}_{i;t;1;\uparrow}\psi^{\dagger}_{i;b;1;\downarrow}-\psi^{\dagger}_{i;t;1;\downarrow}\psi^{\dagger}_{i;b;1;\uparrow}+\text{H.c.}) \\ & -\mu_{f}\sum_{l,\sigma,i}f^{\dagger}_{i;l;a;\sigma}f_{i;l;a;\sigma}-\sum_{a=1,2}\mu_{a}\sum_{l,\sigma,i}\psi^{\dagger}_{i;l;a;\sigma}\psi_{i;l;a;\sigma} \end{aligned} \tag{B4}$$

with the coefficients

$$\begin{aligned} & t_{\psi;11}=t^{x}_{\parallel}\left[\tfrac{3}{8}\chi_{f}\chi_{\psi;22}-\tfrac{9}{16}\Phi^{0}_{2}\Phi^{0}_{2}\right]+\tfrac{3}{8}J^{dd}_{\parallel}\chi_{\psi;11}, \\ & t_{\psi;22}=t^{x}_{\parallel}\left[\tfrac{3}{8}\chi_{f}\chi_{\psi;11}\right]+\tfrac{3}{8}J^{dd}_{\parallel}\chi_{\psi;22},\quad t_{f;2}=t^{x}_{\parallel}\left[\tfrac{3}{8}(\chi_{\psi;11}\chi_{\psi;22})\right],\quad C^{0}_{2}=t^{x}_{\parallel}\left[-\tfrac{9}{8}\Phi^{0}_{2}\chi_{\psi;11}\right], \\ & t^{\perp}_{\psi;11}=\tfrac{3}{8}J^{dd}_{\perp}\chi_{\psi;11},\quad t^{\perp}_{\psi;22}=\tfrac{3}{8}J^{dd}_{\perp}\chi_{\psi;22},\quad t^{\perp}_{f}=\tfrac{3}{8}J^{z}_{\perp}\chi^{\perp}_{f},\quad C^{\perp}_{2}=\tfrac{3}{8}J^{sd}_{\perp}\Phi^{\perp}_{2}, \end{aligned}$$

and

$$D_{\psi;1}=\tfrac{3}{8}J^{dd}_{\parallel}\Delta_{\psi;1},\quad D^{\perp}_{\psi;1}=\tfrac{3}{8}J^{dd}_{\perp}\Delta^{\perp}_{\psi;1}.$$

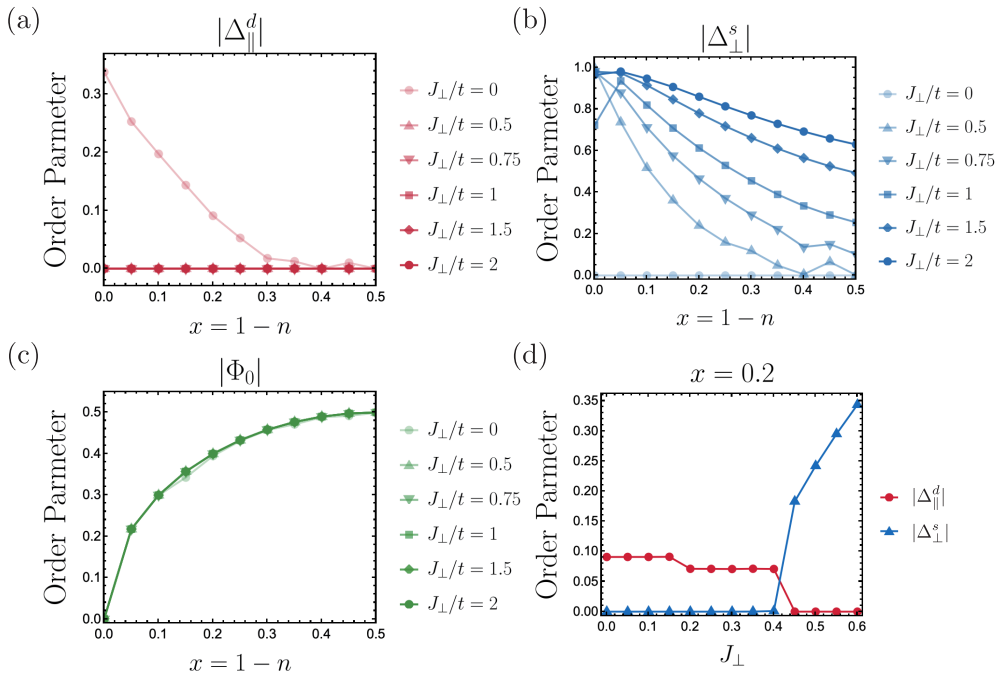

FIG. 5. Mean-field order parameters of the type II t-J model at $t_\parallel^x = 1$. [(a)–(c)] Doping ratio x dependence of intralayer pairing, interlayer pairing, Kondo-like coupling at $J_\parallel^x = 1/2$, (d) interlayer coupling $J_\perp$ dependence of pairings at $x = 0.2$.

There are ten mean-field order parameters in total for constructing a mean-field Hamiltonian,

$$\chi_{\psi;aa} = \sum_\sigma \langle \psi^\dagger_{j;l;a;\sigma} \psi_{i;l;a;\sigma} \rangle, \quad \chi_f = \sum_\sigma \langle f^\dagger_{j;l;2;\sigma} f_{i;l;2;\sigma} \rangle, \quad \Phi_2^0 = \sum_\sigma \langle \psi^\dagger_{i;l;2;\sigma} f_{i;l;2;\sigma} \rangle, \tag{B5}$$

$$\chi^\perp_{\psi;aa} = \sum_\sigma \langle \psi^\dagger_{i;t;a;\sigma} \psi_{i;b;a;\sigma} \rangle, \quad \chi_f^\perp = \sum_\sigma \langle f^\dagger_{i;t;2;\sigma} f_{i;b;2;\sigma} \rangle, \quad \Phi_2^\perp = \sum_\sigma \langle \psi^\dagger_{i;t;2;\sigma} f_{i;b;2;\sigma} \rangle, \tag{B6}$$

$$\Delta_{\psi;1} = \langle s^{ij} (\psi_{i;l;1;\uparrow} \psi_{j;l;1;\downarrow} - \psi_{i;l;1;\downarrow} \psi_{j;l;1;\uparrow}) \rangle, \quad \Delta^\perp_{\psi;1} = \langle \psi_{i;t;1;\uparrow} \psi_{j;b;1;\downarrow} - \psi_{i;t;1;\downarrow} \psi_{j;b;1;\uparrow} \rangle. \tag{B7}$$

Note that $t_{\psi;12} = C_1^0 = C_1^\perp = \chi_{\psi;12} = \Phi_1^0 = \Phi_1^\perp = 0$, and $J_{sd}^\parallel = \frac{1}{2} J_\parallel^x, J_{sd}^\perp = \frac{1}{2} J_\perp^z, J_{dd}^\parallel = \frac{1}{4} J_\parallel^x, J_{dd}^\perp = \frac{1}{4} J_\perp^z$. Together with the order parameters, one should impose the constraints on the number of fermion $n_{\psi;1} = n_{\psi;1} = 1 - x$, and $n_f = x$, where the particle numbers are defined as

$$n_{\psi;a} = \sum_{k,l} \langle \psi^\dagger_{k;l;a;\sigma} \psi_{k;l;a;\sigma} \rangle, \quad n_f = \sum_{k,l} \langle f^\dagger_{k;l;2;\sigma} f_{k;l;2;\sigma} \rangle.$$

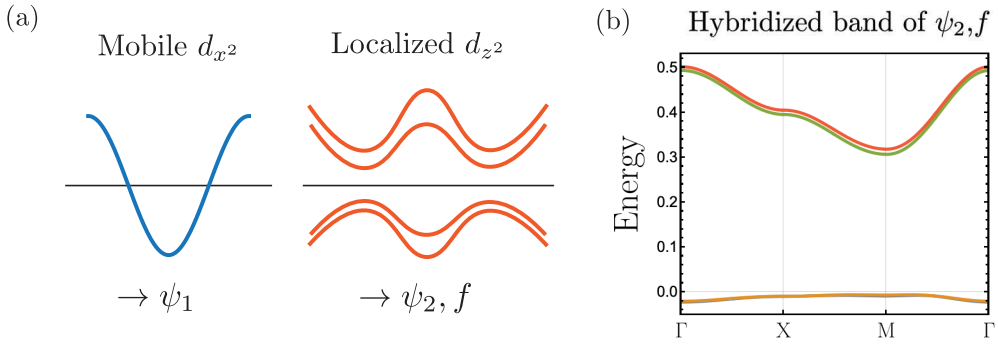

FIG. 6. (a) Schematic illustrations for physical meaning of three fermions. ψ_1 itself means a d_1 orbital, while ψ_2,f together form a localized d_2 orbital. (b) Energy dispersion of localized d_2 sector. We plot the dispersion of the hybridized band of ψ_2,f for justifying that this sector forms a band insulator in mean field level, indicating a gapped rung-singlet phase. For an illustration, we set $J_\perp = 1/2, x = 0.1$.

In Fig. 5, we plot $(\Delta^{\parallel}_{\psi;1}, \Delta^{\perp}_{\psi;1}, \Phi^0_2)$ upon doping with a fraction x of holes. Moreover in Fig. 6, we illustrate the physical meaning of the three fermions in our parton construction. With a non-zero $\Phi = \Phi^0_2$, the ψ_1 orbital can be identified as the d_1 orbital from Eq. (B3). At the same time, ψ_2,f together form a localized d_2 orbital with total density $n_{i;2} + n_{i;f} = 1$ per site. In our bilayer model they form a gapped rung-singlet phase.

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