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Phys. Rev. B **108**, 174511 — Published 21 November 2023

DOI: 10.1103/PhysRevB.108.174511

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

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(Dated: October 19, 2023)

Recently, an 80 K superconductor was discovered in $La_3Ni_2O_7$ under high pressure. Density function theory (DFT) 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 inter-layer super-exchange $J_\perp$ 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 inter-layer 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. Our calculations demonstrate that the pairing strength decreases with the hole doping x and $x = 0.5$ is likely larger than the optimal doping. We propose future experiments to electron dope the system to further enhance T_c.

Introduction: Recently a superconductor with T_c = 80K 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 inter-layer 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 intra-layer 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 inter-layer 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 inter-layer spin coupling $J_\perp$ but without inter-layer 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 inter-layer pairing. The pairing strength decreases with the hole doping level x. 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 inter-layer 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 pro-

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posed 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 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 inter-layer pairing at $x = 0.5$ similar to the one-orbital t-J model before.

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,

$$\begin{aligned} H &= H_K + J^x_\parallel \sum_l \sum_{\langle ij\rangle} \vec{S}_{i;l;1}\cdot\vec{S}_{i;l;1} + J^z_\perp \sum_i \vec{S}_{i;t;2}\cdot\vec{S}_{i;b;2} \\ &+ U'\sum_i n_{i;1}n_{i;2} - 2J_H \sum_i (\vec{S}_{i;l;1}\cdot\vec{S}_{i;l;2} + \frac{1}{4} n_{i;1}n_{i;2}) \end{aligned} \tag{1}$$

and

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

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 $t^x_\parallel = 0.485$, $t^z_\parallel = 0.110$, $t^{xz}_\parallel = 0.239$, $t^z_\perp = 0.635$ by DFT[6]. $s_{ij} = 1$ for the x bond and $s_{ij} = -1$ for the y bond. For simplicity, we only keep intra-layer $J^x_\parallel$ for the $d_{x^2-y^2}$ orbital and the inter-layer $J^z_\perp$ 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 $n_2 \approx 1$.

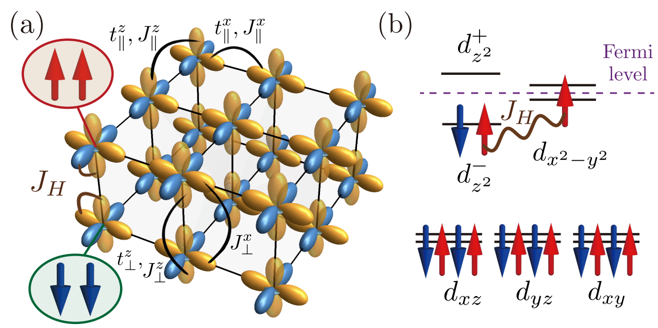

FIG. 1. **(a) The schematics of the bilayer two-orbital model.** The various t, J's are introduced for the hoppings and interactions of two orbitals on square lattices. Importantly, a strong ferromagnetic Hund coupling J_H transmits $J^z_\perp$ of the d_{z^2} orbital to the $d_{x^2-y^2}$ orbital, by 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 $n_2 \simeq 1$.

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 inter-layer spin-spin coupling $J^z_\perp$ also induces anti-ferromagnetic coupling of the d_1 orbital (see the Inset of Fig. 1(a)). Basically only the orbital symmetric part, $J^x_\perp = J^z_\perp$, can persist in the restricted Hilbert space. Consequently, we should consider a significant inter-layer $J_\perp$ also for the $d_{x^2-y^2}$ orbital, though there is no inter-layer hopping.

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

$$\begin{aligned} H_{\text{eff}} &= -t^x_\parallel \sum_{l,\sigma}\sum_{\langle i,j\rangle} P\left(d^\dagger_{i;1;l,\sigma} d_{1;1;l;\sigma}\right) P + H.c. \\ &+ J^x_\parallel \sum_l \sum_{\langle i,j\rangle} \vec{S}_{i;l;1}\cdot\vec{S}_{j;l;1} + J^z_\perp \sum_i \vec{S}_{i;t;1}\cdot\vec{S}_{i;b;1} \end{aligned} \tag{2}$$

Hereafter, shorthand notation $t = t^x_\parallel, J_\parallel = J^x_\parallel$, and $J_\perp = J^z_\perp$ 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 inter-layer 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,

$d^\dagger_{i;l;1;\sigma} = f^\dagger_{i;l;\sigma} b_{i;l}$ with the constraint $n_{i;l;f} + n_{i;l;b} = 1$ (see the Supplemental Material (SM) for details). In mean-field level, we decouple the following order parameters from the J terms: the hopping terms $\chi^l_{\parallel;ij,\sigma} = 2\langle f^\dagger_{i;l;\sigma} f_{j;l;\sigma}\rangle$, $\chi_{\perp;i;\sigma} = 2\langle f^\dagger_{i;t;\sigma} f_{i;b;\sigma}\rangle$ and the pairing terms $\Delta^l_{\parallel;ij} = 2s^{ij}\langle f_{i;l;\uparrow} f_{j;l;\downarrow}\rangle$, $\Delta_{\perp;i} = 2\langle f_{i;t;\uparrow} f_{i;b,\downarrow}\rangle$. 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 $0 \le x \le 1/2$.

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 pairing with dominated inter-layer pairing, as illustrated in Fig.2 (a-b). In Fig.2 (c), we find a first-order transition from the d-wave to s-wave pairing with dominated inter-layer 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 super-exchange of the d_2 orbital which has a large inter-layer coupling. Thus we expect an s-wave inter-layer 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 inter-layer 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.S1 in SM, we show that a large $t_\perp$ term suppresses the pairing because the hopping disfavors inter-layer 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.

Type II t-J model: The importance of Hund's coupling in sharing the super-exchange 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 localized and forms 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 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

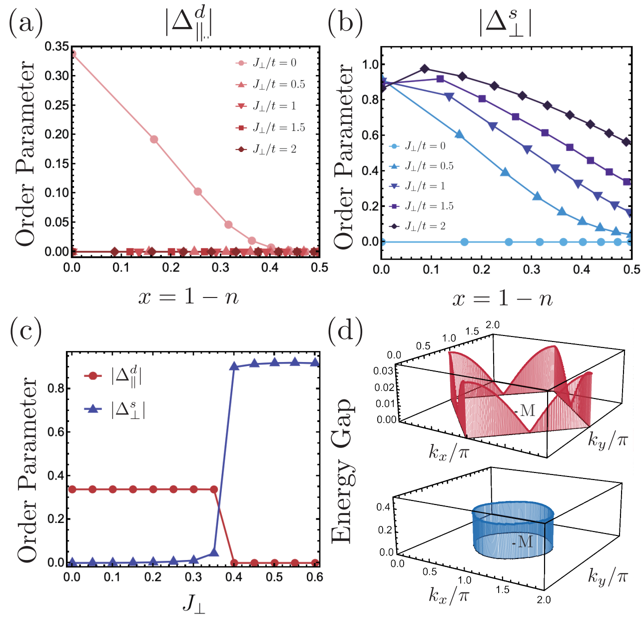

FIG. 2. **(a-b) Zero temperature mean-field solutions of one-orbital t-J model.** We plot the filling x dependence of (a) intra-layer d-wave pairing, (b) inter-layer s-wave pairing within the slave-boson framework are shown at $t^x_\parallel = 1$, $J^x_\parallel = 1/2$. **(c) $J_\perp$ dependence of 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 M=(π,π) point, is completely gapped with a s-wave pairing (bottom), while there are four point nodes with a d-wave pairing (top).

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 is penalized by a large J_H and is removed from the Hilbert space.

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

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

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

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

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.

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 $|a\sigma\rangle_i = f^{\dagger}_{i;a\sigma}|0\rangle$, while the three S=1 doublons are created by $|-1\rangle_i = \psi^{\dagger}_{i;1\downarrow}\psi^{\dagger}_{i;2\downarrow}|0\rangle$, $|0\rangle_i = \frac{1}{\sqrt{2}}(\psi^{\dagger}_{i;1\uparrow}\psi^{\dagger}_{i;2\downarrow} - \psi^{\dagger}_{i;2\uparrow}\psi^{\dagger}_{i;1\downarrow})|0\rangle$ and $|1\rangle = \psi^{\dagger}_{i;1\uparrow}\psi^{\dagger}_{i;2\uparrow}|0\rangle$. 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 $n_{i;f} = \sum_{a\sigma}f^{\dagger}_{i;a\sigma}f_{i;a\sigma}$ and $n_{i;\psi_a} = \sum_\sigma\psi^{\dagger}_{i;a\sigma}\psi_{i;a\sigma}$. 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 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, $d_{i;a\sigma} = \epsilon_{ab}f^{\dagger}_{i;b\sigma}\psi_{i;2\sigma}\psi_{i;1\sigma} + \frac{1}{2}\epsilon_{ab}f^{\dagger}_{i;b\bar{\sigma}}(\psi_{i;2\downarrow}\psi_{i;1\uparrow} + \psi_{i;2\uparrow}\psi_{i;1\downarrow})$. Here, ϵ_{ab} is the anti-symmetric tensor with $\epsilon_{12} = 1$ and $\bar{\sigma}$ denotes the opposite spin of σ. The singlon and doublon spin operators are now represented as, $\vec{s}_{i;a} = \frac{1}{2}\sum_{\sigma,\sigma'}f^{\dagger}_{i;a\sigma}\vec{\sigma}_{\sigma\sigma'}f_{i;a\sigma'}$ and $\vec{S}_i = \frac{1}{2}\sum_a\sum_{\sigma\sigma'}\psi^{\dagger}_{i;a\sigma}\vec{\sigma}_{\sigma\sigma'}\psi_{i;a\sigma'}$.

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 SM. In principle, one can have a phase diagram from tuning Δ and x. For simplicity, we her 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, $\langle\psi^{\dagger}_{i;l;a\sigma}f_{i;l;2\sigma}\rangle = \frac{3}{4}\Phi_a$ 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 $\langle\psi^{\dagger}_{i;l;2\sigma}f_{i;l;2\sigma}\rangle = 3\Phi_2/4 \neq 0$ 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 $d_{i;l_1\sigma} \sim \frac{3}{4}\Phi_2^{\dagger}\psi_{i;l;1\sigma}$,

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

where $\vec{S}_{i;l;\psi_1} = \frac{1}{2}\psi^{\dagger}_{i;l;1\sigma}\vec{\sigma}_{\sigma\sigma'}\psi_{i;l;1\sigma'}$ 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 super-exchange 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 inter-layer 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 S2(c) in SM).

We perform a full 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 intra-layer and inter-layer pairing terms as shown in Fig. 3(a-b). Note that we still use t, $J_{\parallel}$, and $J_{\perp}$ as abbreviation 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 inter-layer pairing (See Fig.S2(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 Fig. 2(a-b)), justifying our previous treatment. However, now we achieve these results from a more precise approach of a

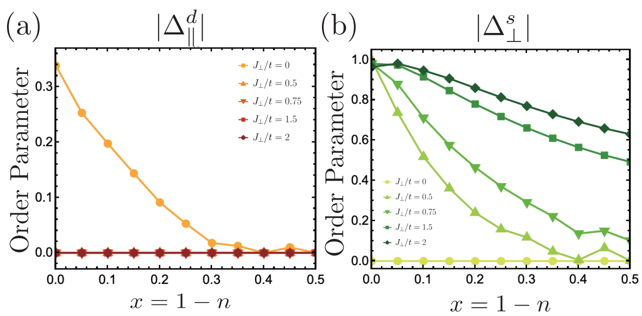

FIG. 3. **(a-b) Zero temperature mean-field solutions of type II t-J model in the large Δ limit.** We plot the filling x dependence of (a) intra-layer pairing, (b) inter-layer pairing of the emergent '$d_{x^2-y^2}$' orbital at $t_{\parallel}^{x} = 1$, $J_{\parallel}^{x} = 1/2$. Comparing 2(a-b) and 3(a-b), 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.

microscopic model. The sharing of the super-exchange of one orbital to the other orbital is automatically taken care of in our model and parton framework.

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 super-exchange 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 can not 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 inter-layer 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 1D 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 $La_3Ni_2O_7$.

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 super-exchange 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 inter-layer hopping, but with enhanced inter-layer anti-ferromagnetic spin-spin coupling $J_{\perp}$ over intra-layer hopping t. Mean field theory then predicts a s-wave inter-layer paired superconductor even at hole doping 50%, in agreement with the experiment. In 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. We also propose future experiments to reduce x through electron doping to search for an even higher T_c than 80 K.

Note added: When finalizing the manuscript, we become aware of a preprint[23] which also studied a bilayer one-orbital t-J model with strong inter-layer $J_{\perp}$, 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 the 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.

Acknowledgement: YHZ was supported by the National Science Foundation under Grant No. DMR-2237031.

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Appendix A: One-orbital t-J model and slave-boson theory

We start from the one-orbital Hamiltonian,

$$\begin{aligned} H = &-t_{\parallel}^{x}\sum_{l,\sigma}\sum_{\langle i,j\rangle}P\left(d^{\dagger}_{i;1;l,\sigma}d_{1;l;\sigma}\right)P + H.c.\\ &+ J_{\parallel}^{x}\sum_{l}\sum_{\langle i,j\rangle}\vec{S}_{i;l;1}\cdot\vec{S}_{i;l;1} + J_{\perp}^{z}\sum_{i}\vec{S}_{i;t;1}\cdot\vec{S}_{i;b;1}, \end{aligned} \tag{S1}$$

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

$$\begin{aligned} H_{SB}^{MF} \;=\; &-t_{\parallel}\sum_{l,\sigma,\langle i,j\rangle}\left(f^{\dagger}_{i;l;\sigma}f_{j;l;\sigma} + h.c.\right) - t_{\perp}\sum_{\sigma,i}\left(f^{\dagger}_{i;t;\sigma}f_{i;b;\sigma} + h.c.\right)\\ &+D_{\parallel}\sum_{l,\langle i,j\rangle}\left(s_{ij}(f^{\dagger}_{i;l;1;\uparrow}f^{\dagger}_{j;l;1;\downarrow} - f^{\dagger}_{i;l;1;\downarrow}f^{\dagger}_{j;l;1;\uparrow}) + h.c.\right)\\ &+D_{\perp}\sum_{i}\left(f^{\dagger}_{i;t;\uparrow}f^{\dagger}_{i;b;\downarrow} - f^{\dagger}_{i;t;\downarrow}f^{\dagger}_{i;b;\uparrow} + h.c.\right), \end{aligned} \tag{S2}$$

with the coefficients,

$$\begin{aligned} t_{\parallel} &= xt_{\parallel}^{x} + \frac{3}{8}J_{\parallel}^{x}\chi_{\parallel}, \quad t_{\perp} = \frac{3}{8}J_{\perp}^{z}\chi_{\perp},\\ D^{\parallel} &= \frac{3}{8}J_{\parallel}^{x}\Delta_{\parallel}^{d}, \quad D^{\perp} = \frac{3}{8}J_{\perp}^{z}\Delta_{\perp}^{s}. \end{aligned}$$

There are 4 mean field order parameters,

$$\chi_{\parallel} \;=\; \sum_{\sigma}\langle f^{\dagger}_{j;l;\sigma}f_{i;l;\sigma}\rangle, \quad \chi_{\perp} = \sum_{\sigma}\langle f^{\dagger}_{i;t;\sigma}f_{i;b;\sigma}\rangle, \tag{S3}$$

$$\Delta_{\parallel} = \langle s^{ij}(f_{i;l;\uparrow}f_{j;l;\downarrow} - f_{i;l;\downarrow}f_{j;l;\uparrow})\rangle, \quad \Delta_{\perp} = \langle f_{i;t;\uparrow}f_{j;b;\downarrow} - f_{i;t;\downarrow}f_{j;b;\uparrow}\rangle. \tag{S4}$$

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

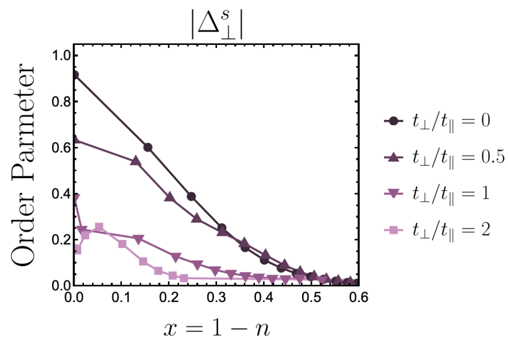

FIG. S1. **Mean-field order parameters of the one-orbital model.** Inter-layer hopping $t_{\perp}$ dependence of the inter-layer pairing at $J_{\perp} = 1/2$. The inclusion of larger inter-layer hopping $t_{\perp}$ suppressed the inter-layer pairing order parameter $\Delta_{\perp}$.

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,

$$\begin{aligned} H &= -t^{x}_{\parallel}\sum_{l,\sigma,\langle i,j\rangle}(P_0 d^{\dagger}_{i;l;1;\sigma}d_{j;l;1;\sigma}P_0 + h.c.) \\ &+J^{x}_{\parallel}\sum_{l,\langle i,j\rangle}\vec{s}_{i;l;1}\cdot\vec{s}_{j;l;1} + J^{dd}_{\parallel}\sum_{l,\langle i,j\rangle}\vec{S}_{i;l}\cdot\vec{S}_{j;l} + J^{sd}_{\parallel}\sum_{l,\langle i,j\rangle}(\vec{s}_{i;l;1}\cdot\vec{S}_{j;l} + \cdot\vec{S}_{i;l}\cdot\vec{s}_{j;l;1}) \\ &+J^{z}_{\perp}\sum_{i}\vec{s}_{i;t;2}\cdot\vec{s}_{i;b;2} + J^{dd}_{\perp}\sum_{i}\vec{S}_{i;t}\cdot\vec{S}_{i;b} + J^{sd}_{\perp}\sum_{i}(\vec{s}_{i;t;2}\cdot\vec{S}_{i;b} + \vec{S}_{i;t}\cdot\vec{s}_{i;b;2}) \end{aligned} \tag{S1}$$

Here we use the following three-fermion decomposition,

$$d^{\dagger}_{i;l;1;\sigma} = (\psi^{\dagger}_{i;l;1;\sigma}\psi^{\dagger}_{i;l;2;\sigma})f_{i;l;2;\sigma} + \frac{1}{2}(\psi^{\dagger}_{i;l;1\uparrow}\psi^{\dagger}_{i;2;l;\downarrow} + \psi^{\dagger}_{i;1;l;\downarrow}\psi^{\dagger}_{i;2;l;\uparrow})f_{i;l;2;\bar{\sigma}}, \tag{S2}$$

$$d_{j;l;1;\sigma} = f^{\dagger}_{j;l;2;\sigma}(\psi_{j;l;2;\sigma}\psi_{j;l;1;\sigma}) + \frac{1}{2}f^{\dagger}_{j;l;2;\bar{\sigma}}(\psi_{j;l;2;\downarrow}\psi_{j;l;1;\uparrow} + \psi_{j;l;2;\uparrow}\psi_{j;l;1;\downarrow}). \tag{S3}$$

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

$$\begin{aligned} H^{MF}_{TF} &= -t_{f;2}\sum_{l,\sigma,\langle i,j\rangle}\left(f^{\dagger}_{i;l;2;\sigma}f_{j;l;2;\sigma} + h.c.\right) - \sum_{a,c=1,2}t_{\psi;ac}\sum_{l,\sigma,\langle i,j\rangle}\left(\psi^{\dagger}_{i;l;a;\sigma}\psi_{j;l;c;\sigma} + h.c.\right) \\ &- \sum_{a=1,2}C^{0}_{a}\sum_{l,\sigma,i}\left(f^{\dagger}_{i;l;2;\sigma}\psi_{i;l;a;\sigma} + \psi^{\dagger}_{i;l;a;\sigma}f_{i;l;2;\sigma} + h.c.\right) \\ &-t^{\perp}_{f}\sum_{\sigma,i}\left(f^{\dagger}_{i;t;2;\sigma}f_{i;b;2;\sigma} + h.c.\right) - \sum_{a,c=1,2}t^{\perp}_{\psi;ac}\sum_{\sigma,i}\left(\psi^{\dagger}_{i;t;a;\sigma}\psi_{i;b;c;\sigma} + h.c.\right) \\ &- \sum_{a=1,2}C^{\perp}_{a}\sum_{\sigma,i}\left(f^{\dagger}_{i;t;2;\sigma}\psi_{i;b;a;\sigma} + \psi^{\dagger}_{i;t;a;\sigma}f_{i;b;2;\sigma} + h.c.\right) \\ &+D_{\psi;1}\sum_{l,\langle i,j\rangle}\left(s_{ij}(\psi^{\dagger}_{i;l;1;\uparrow}\psi^{\dagger}_{j;l;1;\downarrow} - \psi^{\dagger}_{i;l;1;\downarrow}\psi^{\dagger}_{j;l;1;\uparrow}) + h.c.\right) \end{aligned} \tag{S4}$$

$$
\begin{aligned}
&+D^{\perp}_{\psi;1}\sum_i\left(\psi^\dagger_{i;t;1;\uparrow}\psi^\dagger_{i;b;1;\downarrow}-\psi^\dagger_{i;t;1;\downarrow}\psi^\dagger_{i;b;1;\uparrow}+h.c.\right)\\
&-\mu_f\sum_{l,\sigma,i}f^\dagger_{i;l;a;\sigma}f_{i;l;a;\sigma}-\sum_{a=1,2}\mu_a\sum_{l,\sigma,i}\psi^\dagger_{i;l;a;\sigma}\psi_{i;l;a;\sigma},
\end{aligned}
$$

with the coefficients,

$$
\begin{aligned}
t_{\psi;11} &= t^x_\parallel\left[\frac{3}{8}\chi_f\chi_{\psi;22}-\frac{9}{16}\Phi^0_2\Phi^0_2\right]+\frac{3}{8}J^{dd}_\parallel\chi_{\psi;11},\\
t_{\psi;22} &= t^x_\parallel\left[\frac{3}{8}\chi_f\chi_{\psi;11}\right]+\frac{3}{8}J^{dd}_\parallel\chi_{\psi;22},\quad t_{f;2}=t^x_\parallel\left[\frac{3}{8}\left(\chi_{\psi;11}\chi_{\psi;22}\right)\right],\quad C^0_2=t^x_\parallel\left[-\frac{9}{8}\Phi^0_2\chi_{\psi;11}\right],\\
t^\perp_{\psi;11} &= \frac{3}{8}J^{dd}_\perp\chi_{\psi;11},\quad t^\perp_{\psi;22}=\frac{3}{8}J^{dd}_\perp\chi_{\psi;22},\quad t^\perp_f=\frac{3}{8}J^z_\perp\chi^\perp_f,\quad C^\perp_2=\frac{3}{8}J^{sd}_\perp\Phi^\perp_2,
\end{aligned}
$$

and

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

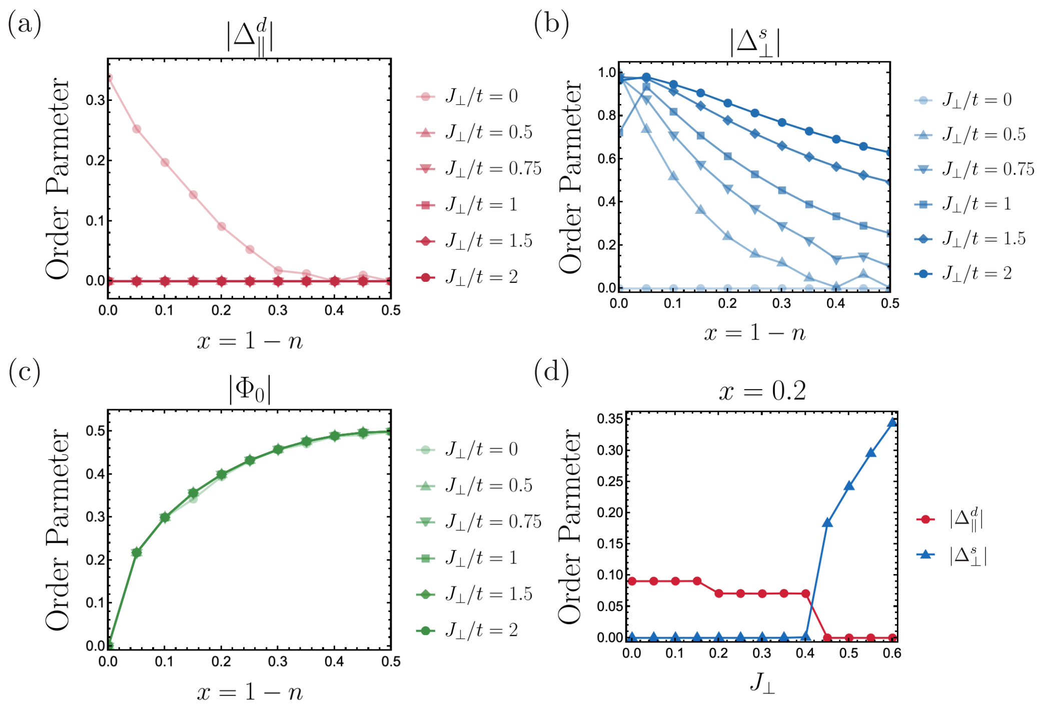

FIG. S2. **Mean-field order parameters of the type II t-J model** at $t^x_\parallel=1$. (a-c) Doping ratio x dependence of intra-layer pairing, inter-layer pairing, Kondo-like coupling at $J^x_\parallel=1/2$, (d) Inter-layer coupling $J_\perp$ dependence of pairings at $x=0.2$.

There are 10 mean-field order parameters in total for constructing a mean-field Hamiltonian,

$$
\chi_{\psi;aa} = \sum_\sigma\langle\psi^\dagger_{j;l;a;\sigma}\psi_{i;l;a;\sigma}\rangle,\quad \chi_f=\sum_\sigma\langle f^\dagger_{j;l;2;\sigma}f_{i;l;2;\sigma}\rangle,\quad \Phi^0_2=\sum_\sigma\langle\psi^\dagger_{i;l;2;\sigma}f_{i;l;2;\sigma}\rangle, \tag{S5}
$$

$$
\chi^\perp_{\psi;aa} = \sum_\sigma\langle\psi^\dagger_{i;t;a;\sigma}\psi_{i;b;a;\sigma}\rangle,\quad \chi^\perp_f=\sum_\sigma\langle f^\dagger_{i;t;2;\sigma}f_{i;b;2;\sigma}\rangle,\quad \Phi^\perp_2=\sum_\sigma\langle\psi^\dagger_{i;t;2;\sigma}f_{i;b;2;\sigma}\rangle, \tag{S6}
$$

$$
\Delta_{\psi;1} = \langle s^{ij}(\psi_{i;l;1;\uparrow}\psi_{j;l;1;\downarrow}-\psi_{i;l;1;\downarrow}\psi_{j;l;1;\uparrow})\rangle,\quad \Delta^\perp_{\psi;1}=\langle\psi_{i;t;1;\uparrow}\psi_{j;b;1;\downarrow}-\psi_{i;t;1;\downarrow}\psi_{j;b;1;\uparrow}\rangle. \tag{S7}
$$

Note that $t_{\psi;12}=C^0_1=C^\perp_1=\chi_{\psi;12}=\Phi^0_1=\Phi^\perp_1=0$, and $J^\parallel_{sd}=\frac{1}{2}J^x_\parallel$, $J^\perp_{sd}=\frac{1}{2}J^z_\perp$, $J^\parallel_{dd}=\frac{1}{4}J^x_\parallel$, $J^\perp_{dd}=\frac{1}{4}J^z_\perp$. 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,

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

In Fig.S2, we plot $(\Delta^{\parallel}_{\psi;1}, \Delta^{\perp}_{\psi;1}, \Phi^0_2)$ upon doping with a fraction x of holes. Moreover in Fig.S3, 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. S3. 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.

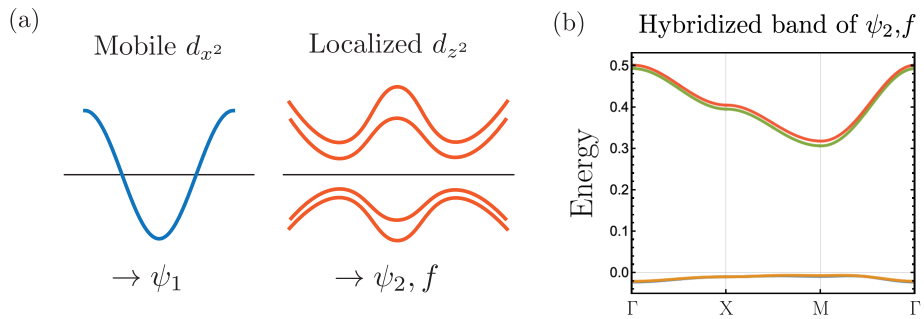

FIG. S3. **(a)Schematic illustrations for physical meaning of three fermions.** ψ_1 itself means a d_1 orbital, while ψ_2,f together form a localized d_2 orbital. **(b) Energy dispersion of localized d_2 sector.** We plot the dispersion of the hybridized band of ψ_2,f for justifying that this sector forms a band insulator in mean field level, indicating a gapped rung-singlet phase. For an illustration, we set $J_\perp = 1/2, x = 0.1$.