Type-II t-J model in superconducting nickelate $Nd_{1-x}Sr_xNiO_2$

Ya-Hui Zhang and Ashvin Vishwanath
Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

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The recent observation of superconductivity at relatively high temperatures in hole-doped $NdNiO_2$ has generated considerable interest, particularly due to its similarity with the infinite layer cuprates. Building on the observation that the Ni^{2+} ions resulting from hole doping are commonly found in the spin-triplet state, we introduce and study a variant of the t-J model in which the holes carry $S = 1$. We name this model the type-II t-J model. We find two distinct mechanisms for d-wave superconductivity. In both scenarios the pairing is driven by the spin coupling J. However, coherence is gained in distinct ways in these two scenarios. In the first case, the spin-one holes condense, leading to a d-wave superconductor along with spin-symmetry breaking. Different orders, including spin-nematic orders, are possible. This scenario is captured by a spin-one slave boson theory. In the second scenario, a coherent and symmetric d-wave superconductor is achieved from "Kondo resonance": spin-one holes contribute two electrons to form a large Fermi surface together with the spin-1/2 singly occupied sites. The large Fermi surface then undergoes d-wave pairing because of spin coupling J, similar to heavy fermion superconductors. We propose a three-fermion parton theory to treat these two different scenarios in one unified framework and calculate its doping phase diagram within a self-consistent mean-field approximation. Our study shows that a combination of "cuprate physics" and "heavy fermion physics" may emerge in the type-II t-J model.

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I. INTRODUCTION

Recently, a tour de force materials synthesis effort created a thin film of the hole-doped infinite-layer nickelate $NdNiO_2$ [1]. In this material, the uncommon Ni^{1+} in the $3d^9$ configuration is realized, similar to Cu^{2+} in the high-T_c cuprate materials. Remarkably, a relatively high superconducting transition temperature $T_c \approx 9$–15 K was reported [1]. Besides, according to LDA + U calculations [2–11], the band at Fermi level is dominated by the $d_{x^2-y^2}$ orbital of Ni, which suggests that the main physics may also be governed by a one-band Hubbard model as in the cuprates. However, in this paper we argue that the physics of the hole-doped nickelate is essentially different from that of the cuprates. In cuprates, the near degeneracy of oxygen $2p$ and copper $d_{x^2-y^2}$ orbitals leads to the well-known fact that the doped hole enters the oxygen $2p$ orbital and forms the Zhang-Rice singlet [12]. In contrast, the oxygen $2p$ orbital is far away from the Fermi level in the nickelate due to the lower oxidation state of the Ni^{1+} ion compared to Cu^{2+}. Therefore the doped hole enters the $3d$ orbital and creates a Ni^{2+} state with $3d^8$ configuration. The remaining question is whether the hole is in the low ($S = 0$) or high ($S = 1$) configuration. The Ni^{2+} ion is often found in the high-spin $S = 1$ state [13,14], thanks to Hund's first rule. For example, the spin-one Haldane chain is realized in the Ni^2+, d^8 configuration [15]. In this case, we expect the hole-doped $NdNiO_2$ to likely be described by a novel t-J model with spin-one holes. However, in the absence of a direct experimental measurement of the spin state of the doped hole, one cannot rule out the possibility that Ni^{2+} is in the low-spin state because of a larger energy splitting of the two e_g orbitals. Indeed, such a low spin configuration was proposed in a different but related compound [16] based on certain spectroscopic measurements, although more data may be needed to confirm the conclusion. In this case one must revert to a cupratelike t-J model [14,17–20], at least as far as doped holes are concerned. In this paper we study the unconventional t-J model with spin-one holes, which we dub the type-II t-J model. This model is of theoretical interest even as its relevance to the hole-doped $NdNiO_2$ awaits experimental confirmation. Besides, we hope our theoretical analysis will motivate more experimental searches for realizing this type-II t-J model. Doping electrons into the $3d^7$ configuration is also promising in this regard.

II. TYPE-II t-J MODEL

Let us sketch the form of the type-II t-J model; more details on the derivation from the microscopic Hubbard Hamiltonian can be found in the Appendixes. For convenience, we use the hole picture in this paper and define the vacuum as the $3d^{10}$ state for each site, describing the particle-hole transformed version of the original problem. In this picture, the undoped parent compound has a single hole on each site, which we call a *singlon*, while the state with two holes obtained on doping is called a *doublon*. The doped hole enters the d_{z^2} orbital and creates a doubly occupied site with two holes sitting on the

two e_g orbitals. Because of the interorbital Hund's coupling, the two holes form a spin-triplet ($S = 1$) state. We assume that the singlon is always on the $d_{x^2-y^2}$ orbital because of the splitting between the two e_g orbitals. Then the Hilbert space at each site consists of two singlon states and three doublon states. We label the spin-1/2 singlon with $\sigma = \uparrow, \downarrow$ and label the triplet doublon with $a = x, y, z$. We also define a density operator at each site: $n_i = \sum_a |a\rangle \langle a|$. Thus n_i measures the number of doublons and is equal to the number of doped holes. At the doping level x, the density of the singlon and doublon is $1 - x$ and x, respectively, and we have $\langle n_i \rangle = x$.

The physical spin-1/2 and spin-one operators are $S^s_a = \frac{\sigma^a_{\sigma\sigma'}}{2} |\sigma\rangle \langle\sigma'|$ and $S^d_a = -i\epsilon_{abc} |b\rangle \langle c|$, respectively. The hole operator for the $d_{x^2-y^2}$ orbital is zero (i.e., has vanishing matrix elements) in the restricted Hilbert space, and the only hole operator we have is the one corresponding to the d_{z^2} orbital. Microscopically this hole operator $c^\dagger_\sigma$ creates a hole on the d_{z^2} orbital. In the restricted Hilbert space it acts as

$$c_{i;\uparrow} = \prod_{j<i}(-1)^{n_j+1} \frac{1}{\sqrt{2}} (|\uparrow\rangle_i \langle x|_i - i |\uparrow\rangle \langle y|_i - |\downarrow\rangle_i \langle z|_i),$$
$$c_{i;\downarrow} = \prod_{j<i}(-1)^{n_j+1} \frac{1}{\sqrt{2}} (-|\downarrow\rangle_i \langle x|_i - i |\downarrow\rangle \langle y|_i - |\uparrow\rangle_i \langle z|_i), \tag{1}$$

where $\prod_{j<i}(-1)^{n_j+1}$ is the Jordan-Wigner string to enforce fermionic statistics.

In terms of $c_{i;\sigma}$, $n_i = \sum_\sigma c^\dagger_{i;\sigma} c_{i;\sigma}$, $\vec{S}^d_i = \sum_{\sigma,\sigma'} c^\dagger_{i;\sigma} \vec{\sigma}_{\sigma\sigma'} c_{i;\sigma'}$, and $\vec{S}^s_i = \sum_{\sigma,\sigma'} c_{i;\sigma'} \vec{\sigma}_{\sigma\sigma'} c^\dagger_{i;\sigma}$. Meanwhile $c_{i;\sigma} c^\dagger_{i;\sigma} + c^\dagger_{i;\sigma} c_{i;\sigma} = 1$ and $\{c_{i;\uparrow}, c^\dagger_{i;\downarrow}\} = 0$ do not hold anymore. Thus one should be careful in treating $c_{i;\sigma}$ as a conventional electron operator. The anticommutation relation between two operators of different sites still holds.

With the above definition of Hilbert space and physical operators, the type-II t-J model can be written as

$$H_{t\text{-}J} = H_t + H_J, \tag{2}$$

$$H_t = -\sum_{\langle ij\rangle} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}, \tag{3}$$

$$H_J = \sum_{\langle ij\rangle} \Big[J \mathbf{S^s_i} \cdot \mathbf{S^s_j} + J_d \mathbf{S^d_i} \cdot \mathbf{S^d_j} + \frac{J'}{2} \big(\mathbf{S^s_i} \cdot \mathbf{S^d_j} + \mathbf{S^d_i} \cdot \mathbf{S^s_j} \big) - \Big(J_d + \frac{1}{4} J - J' \Big) n_i n_j \Big]. \tag{4}$$

Generically we expect $J' \gtrsim J$. Microscopically t_{ij} is the hopping of the d_{z^2} orbital and thus it has a large value in the z direction [21]. This means that the t-J model for nickelate may need to be viewed as a three-dimensional (3D) model. Here, for simplicity, we will study the two-dimensional (2D) version of the t-J model and leave the 3D theory to future work.

We need to emphasize that the $c_{i\sigma}$ operator in Eq. (4) is defined in the restricted Hilbert space. Even if we set $J = J' = 0$, Eq. (4) does not reduce to a free fermion model. $c_{i\sigma}$ annihilates a doublon state and creates a singlon at the same site. The hopping term in the t-J model is essentially an exchange of singlon and doublon, which are therefore better variables than the electron operator $c_{i\sigma}$ to describe the underlying phases. At the limit $J, J' \to 0$, we expect a ferromagnetic ground state through the double exchange mechanism [22]. However, superexchange terms J, J' should suppress the ferromagnetism above a critical value. We will focus on the region where the J, J' are large enough to favor a paramagnetic or antiferromagnetic ground state.

Intuitively, there are two possible pictures in this t-J model. (1) In the simple picture, we just assume singlon-doublon separation. We can treat the doublon as a spin-one boson and it naturally condenses at finite density x. With the condensation of the doublon, fermionic singlons can move coherently and form Fermi surfaces and then pair because of local antiferromagnetic spin coupling J. This is a simple generalization of the resonating valence bond (RVB) theory [23,24]. However, in our case the condensation of the spin-one doublon necessarily breaks spin rotation symmetry. We call the resulting phases spin-nematic d-wave superconductor (SN-dSC) and spin-nematic Fermi liquid (SN-FL) phases. (2) In our t-J model there is spin coupling J' between the singlon and the doublon. Hence the singlon-doublon separation assumption may not be valid. "Kondo resonance" between singlons and doublons can be induced by J'. One can imagine a "heavy Fermi liquid" phase where each spin-one doublon contributes two particles and forms large Fermi surfaces together with the singlons, similar to "Kondo screening" in heavy fermion systems. Because the doublon carries spin one, Kondo screening from the spin-1/2 singlon happens in two steps. In the first stage, below a larger temperature T^1_K, half of the doublon is screened by the singlons, while the other half forms a small hole pocket. In a certain sense the physics can be understood in the following intuitive way: the doped hole enters the d_{z^2} orbital and forms a small pocket while there is a local spin-1/2 moment sitting on $d_{x^2-y^2}$ orbital at every site. The resulting phase is either a fractionalized Fermi liquid (FL*) or an antiferromagnetic ordered Fermi liquid with small Fermi surfaces. Then in the second stage, the small pocket absorbs the local spin 1/2 to form a large Fermi surface below a Kondo scale T^2_K. Because of spin coupling J, the large Fermi surface gives way to a d-wave superconductor at lower temperature.

In this paper we will show that this Kondo resonance picture can indeed naturally emerge in our t-J model and be described by a parton mean-field theory. The parton theory can also describe the "SN-SC" and "SN-FL" phase from doublon condensation. Therefore we can study both scenarios above within one unified framework. Our mean-field calculation shows that the Kondo resonance scenarios win unless there is a large external spin rotation breaking anisotropy. In the following we first give a brief discussion of the SN-dSC phase through a doublon condensation lens. Then we propose our parton theory to describe both doublon condensation and Kondo resonance phases. A phase diagram based on mean-field calculation is provided.

III. SLAVE BOSON THEORY

We introduce a spin-one slave boson to label the triplet doublon, extending the popular slave boson theory of correlated electrons where the charge-carrying boson is a spin

singlet [24]:

$$c_\uparrow = \frac{1}{\sqrt{2}} f_\uparrow^\dagger (b_x - i b_y) - \frac{1}{\sqrt{2}} f_\downarrow^\dagger b_z ,$$
$$c_\downarrow = -\frac{1}{\sqrt{2}} f_\downarrow^\dagger (b_x + i b_y) - \frac{1}{\sqrt{2}} f_\uparrow^\dagger b_z . \quad (5)$$

$\vec{b} = (b_x, b_y, b_z)$ transforms as a vector under spin $SO(3)$ rotation. The spin operator of the doublon can be written as

$$\vec{S}_i^d = -i \vec{b}_i^\dagger \times \vec{b}_i . \quad (6)$$

The constraint is $n_{b;i} + n_{f;i} = 1$ and $n_{b;i}, n_{f;i} = 0, 1$. On average we have $\langle n_b \rangle = x$ and $\langle n_f \rangle = 1 - x$.

In the mean-field theory, the boson b and fermion f decouple. At finite density x, the bosonic spin-one doublon condenses to a spin-rotation breaking "superfluid" (which, of course, does not immediately imply a physical superfluid, since the slave bosons also carry gauge charge). For example, consider the simple ansatz with $\langle b_x \rangle = 0$. It breaks spin rotation but preserves the time-reversal symmetry. Equation (5) shows that $c_\sigma \sim f_\sigma^\dagger$ and f can now be viewed as an electron operator. Depending on the ansatz for f, we can obtain *either* a d-wave superconductor or a Fermi liquid, with broken $SO(3)$ spin rotation symmetry. In the presence of spin-orbit coupling, the crystal structure will need to be considered to determine if there is actually any lowering of symmetry. The mean-field theory assuming slave boson condensation is exactly the same as that of the conventional t-J model [24], and one expects a d-wave superconducting dome at small x. However, other condensates such as $\langle \vec{b} \rangle = \vec{\psi}_1 + i\vec{\psi}_2$, where $\vec{\psi}_1 \times \vec{\psi}_2 \neq 0$, will correspond to ordered magnetic moments that break time-reversal symmetry. We leave it to future work to determine the details of the symmetry breaking.

IV. THREE-FERMION PARTON THEORY

The spin-one slave boson approach does not include the possibility of Kondo resonance and can only describe FL/SC with spin rotation breaking. In this theory, the singlon and doublon decouple. However, because of the J' term, we expect that the singlon and doublon couple with each other through Kondo resonance. Obviously, we need a framework which can get access to both the Kondo resonance regime and the Kondo breakdown regime. In this section we show that this is possible in a new parton construction. We introduce two spin-1/2 fermions $\Psi_\sigma = (\psi_{1\sigma}, \psi_{2\sigma})^T$ to label the doublon state. We label the doublon states by $|a\rangle = -\frac{1}{2\sqrt{2}} \Psi^\dagger \tau_y \sigma_a \sigma_y (\Psi^\dagger)^T |0\rangle$, where τ is the Pauli matrix in orbital space. In the restricted five-dimensional Hilbert space at each site,

$$c_\uparrow = f_\uparrow^\dagger \psi_{1\uparrow} \psi_{2\uparrow} + \tfrac{1}{2} f_\downarrow^\dagger (\psi_{1\uparrow}\psi_{2\downarrow} + \psi_{1\downarrow}\psi_{2\uparrow}),$$
$$c_\downarrow = f_\downarrow^\dagger \psi_{1\downarrow} \psi_{2\downarrow} + \tfrac{1}{2} f_\uparrow^\dagger (\psi_{1\uparrow}\psi_{2\downarrow} + \psi_{1\downarrow}\psi_{2\uparrow}), \quad (7)$$

under the constraints $n_{f;i} + n_{\psi_1;i} = 1$ and $\Psi_{i,\sigma}^\dagger \tau_a \Psi_{i,\sigma} = 0$. The latter one constrains $\psi_{i;1}, \psi_{i;2}$ to form an orbital singlet, spin triplet at each site. Again, f and ψ_1, ψ_2 are hard-core fermions whose density at each site can only be zero or 1. On average we have $\langle n_f \rangle = 1 - x$ and $\langle \psi_1 \rangle = \langle \psi_2 \rangle = x$.

We can see that the original electron (hole) operator is now written as a combination of three-fermionic parton operators. We dub this parton construction as a "three-fermion parton." A similar construction has been proposed for the $SU(4)$ Hubbard model at total filling $\nu_T = 1 + x$ [25]. There is a $SU(2)$ gauge symmetry: $\Psi_\sigma \to U \Psi_\sigma$ for $U \in SU(2)$. There is another $U(1)$ gauge symmetry shared by f and ψ: $f_i \to f_i e^{i\alpha_i}$ and $\Psi_i \to \Psi_i e^{i\frac{1}{2}\alpha_i}$. We assign the physical change in the way that ψ_1, ψ_2 carries 1/2 charge while f is neutral.

The spin operator is standard:

$$\vec{S}^s = \tfrac{1}{2} f_\alpha^\dagger \vec{\sigma}_{\alpha\beta} f_\beta , \quad (8)$$

and

$$\vec{S}^d = \frac{1}{2} \sum_{a=1,2} \psi_{a,\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{a,\beta} . \quad (9)$$

H_J in the t-J model can be written using the above expressions. We can also rewrite the hopping term t_2 using the three-fermion operators. It is of the form: $f_j^\dagger f_i (\psi_{i;2}^\dagger \psi_{i;1}^\dagger)(\psi_{j;1}\psi_{j;2})$ (see Appendix B for more details).

We can have a mean-field theory by decoupling the original Hamiltonian:

$$\begin{aligned} H_M = & -t_f \sum_{\langle ij \rangle} f_{i\sigma}^\dagger f_{j\sigma} + \text{H.c.} - t_{ab}^\psi \sum_{ab=1,2} \sum_{\langle ij \rangle} \psi_{i;a}^\dagger \psi_{j;b} + \text{H.c.} \\ & - \Phi_a \sum_{\langle ij \rangle} (f_{i\sigma}^\dagger \psi_{j;a\sigma} + \psi_{i;a\sigma}^\dagger f_{j\sigma}) + \text{H.c.} \\ & - \Phi_a^0 \sum_i (f_i^\dagger \psi_{i;a} + \psi_{i;a}^\dagger f_i) \\ & - \mu_f \sum_i n_i^f - \mu_1 \sum_i n_{i;1}^\psi - \mu_2 \sum_i n_{i;2}^\psi \\ & - \mu_x \sum_i (\psi_{i;1}^\dagger \psi_{i;2} + \text{H.c.}) \\ & + \sum_{\langle ij \rangle} \Delta_{f;ij} (f_{i;\uparrow}^\dagger f_{j;\downarrow}^\dagger - f_{i\downarrow}^\dagger f_{j;\uparrow}^\dagger) + \text{H.c.} \\ & + \sum_{\langle ij \rangle} \Delta_{f,\psi_a;ij} (f_{i;\uparrow}^\dagger \psi_{j;a\downarrow}^\dagger - f_{i;\downarrow}^\dagger \psi_{j;a\uparrow}^\dagger) + \text{H.c.} \\ & + \Delta_t \sum_i (\psi_{i;1\uparrow}^\dagger \psi_{i;2\uparrow}^\dagger + \psi_{i;1\downarrow}^\dagger \psi_{i;2\downarrow}^\dagger) + \text{H.c.} \end{aligned} \quad (10)$$

μ_f, μ_1, μ_2 are introduced to fix the density $\langle n_f \rangle = 1 - x$ and $\langle n_{\psi_1} \rangle = \langle n_{\psi_2} \rangle = x$. Meanwhile, we need μ_x to fix the constraint that $\Psi_i^\dagger \tau_{x,y} \Psi_i = 0$.

We have two sets of Kondo-like couplings: (1) Φ_a^0 is on-site and is from the hopping term, while Φ_a is between two nearest-neighbor sites and originates from the J' coupling. By using $SU(2)$ gauge invariance we can remove one of them. Here we choose to fix $\Phi_2^0 = 0$; (2) from J' coupling we also decouple a pairing term $\Delta_{f\psi_a}$. $\Delta_{f\psi_a}$ encodes the Kondo resonance that the singlon f and ψ_a want to form into a Kondo singlet. As we show later, to form a Fermi liquid with large Fermi surface, we need $\Phi_1 \neq 0$ and $\Delta_{f\psi_2} \neq 0$.

We also introduce spin-singlet pairing terms between f and between Ψ. From our mean-field calculation, we find that the spin-singlet pairings are *favored* to be of d-wave form. Meanwhile, we allow for an on-site triplet pairing Δ_t for Ψ, which is decoupled from the hopping term.

Depending on the competition between different order parameters, we can have different phases in this framework. Here we list the most relevant ones in the following (see Appendix. E for more details):

(i) $\Phi_1 \neq 0$ (or $\Phi_1^0 \neq 0$) and $\Delta_{f\psi_2} \neq 0$. We find this solution at small x. Both Φ_1 and $\Delta_{f\psi_2}$ can be viewed as Kondo coupling from the J' term. As we argue below, the resulting phase is a Fermi liquid with large Fermi surfaces (FL). If we further include $\Delta_f \neq 0$, we get a d-wave superconductor (dSC). The gauge fluctuations are completely Higgsed in this case.

(ii) $\Phi_1 \neq 0$, $\Phi_1^0 \neq 0$ while $\Delta_{f\psi_2} = \Phi_2 = 0$. In this case f is only coupled to ψ_1. The f and ψ_1 hybridize to form a band with total filling $n = 1$ per site. ψ_2 can now be identified as the physical hole operator and forms a small hole pocket with carrier density x. Analysis of the gauge field (see Appendix E) shows that f, ψ_1 is neutral and they form a $U(1)$ spin liquid with spinon Fermi surfaces or Z_2 spin liquid with Dirac nodal fermions, depending on whether $\Delta_f = 0$ or not, respectively. The resulting phase is the so-called FL* phase, with a small hole pocket of a Fermi liquid coexisting with a spin liquid [26]. In the FL* phase, there is a deconfined $U(1)$ or Z_2 gauge field, depending on whether there is pairing term for the spinon. The gauge fluctuation is important for the spin sector but does not couple to the Fermi liquid part.

For a fixed set of order parameters in the mean-field theory, we can write down a variational wave function: $|\Psi\rangle = P\,|\tilde{\Psi}\rangle$, where $|\tilde{\Psi}\rangle$ is a Slater determinant fixed by the mean-field theory. At each site, the operator P projects to the five states specified by $f^\dagger_{i;\sigma}\,|0\rangle$ and $(\Psi^\dagger)^T\tau_y\sigma_a\Psi^\dagger\,|0\rangle$. The order parameters in the mean-field theory should be determined by minimizing the energy corresponding to the projected wave function.

In the following we try to determine the order parameters in the level of mean-field theory. As is well known in the standard slave boson theory [24], the calculation based on mean-field treatment without considering the projection can only be qualitatively correct. For quantitative prediction, one may need a more sophisticated numerical method such as a variational Monte Carlo. The focus of this paper is at zero temperature. At finite temperature, mean-field treatment may not be valid due to both thermal and quantum fluctuations, and we leave it to future for studies at finite temperature. From solving the self-consistent equations (shown in the Appendixes), we get a plot of order parameters shown in Fig. 1. The dominant order parameters are Φ_1, $\Delta_{f\psi_2}$, and Δ_f. First let us ignore Δ_f. We want to show that Φ_1 and $\Delta_{f\psi_2}$ are Kondo couplings which merge f, ψ_1, ψ_2 to form a conventional Fermi liquid. We have two $U(1)$ gauge fields: a is shared by f and ψ_a, α parameterizes part of the $SU(2)$ gauge field generated by τ_z. f couples to a, ψ_1 couples to $\frac{1}{2}a + \frac{1}{2}\alpha + \frac{1}{2}A$. Now, ψ_2 couples to $\frac{1}{2}a - \frac{1}{2}\alpha + \frac{1}{2}A$. The condensation of Φ_1 and $\Delta_{f\psi_2}$ locks the gauge fields to be $a = -A$ and $\alpha = -2A$. Then f and ψ_1 couple to $-A$ while ψ_2 couples to A. This means that we can view ψ_2 as physical hole operator while viewing f, ψ_1 as physical electron operator. Let us redefine $\tilde{f}_{i;\sigma} = f^\dagger_{i;\sigma}$ and $\tilde{\psi}_{i;1\sigma} = \psi^\dagger_{i;1\sigma}$. Then $\tilde{f}$, $\tilde{\psi}_1$, ψ_2 are all hole operators and they hybridize together to form a Fermi liquid with large Fermi surfaces, as shown in Fig. 2.

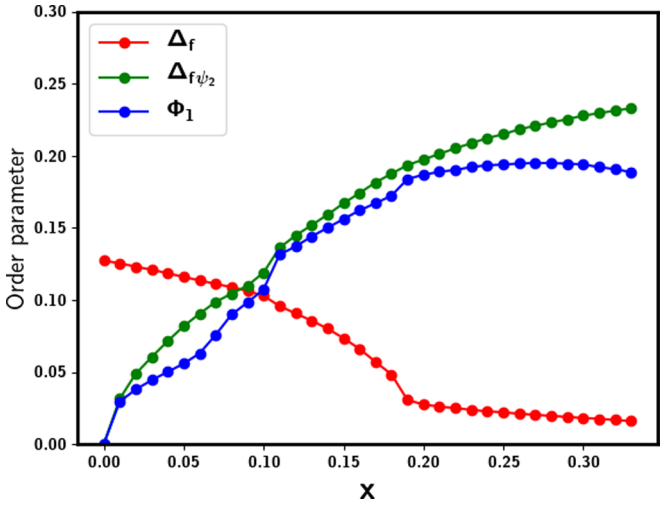

FIG. 1. Mean-field solution from the three-fermion parton mean-field theory using $t = 2J$ and $J' = 4J$. We set $J = 1$ and only show the dominant mean-field amplitudes.

At small x, we find $\Delta_f \neq 0$, and thus the ground state is a d-wave superconductor. Δ_f decreases with doping, resulting a dome similar to that of the cuprates. Here in the under-doped region, T_c is decided by the onset of Φ_1 and $\Delta_{f\psi_2}$. In a certain sense, the destruction of the superconductor is from "Kondo breakdown."

In the above we used $J' = 4J$ to get a stable Fermi liquid or superconductor. For smaller J'/J, there is zero or just one Kondo coupling when $x < x_c$ in the mean-field calculation, resulting in a "pseudogap metals" phase or a FL* phase in the underdoped region. It is not clear whether this is just an artifact of mean-field treatment. Our mean-field theory suggests that the phase diagram at the small x region is like that shown in Fig. 3. One can see that this phase diagram is similar to that from slave boson theory for cuprates [24]. The difference is that here the T_c (or coherence scale) is determined by Kondo breakdown instead of slave boson condensation.

V. ROLE OF Nd ORBITAL

In the undoped sample, resistivity shows metallic behavior above 50 K and an upturn below 50 K. The metallic behavior can be attributed to the electron pocket from the Nd orbital [5–7,17], leading to self-doping. We can extend our t-J model to include the Nd orbital (see the Appendixes):

$$H = H_{t\text{-}J} + \sum_k \xi_{Nd}(\mathbf{k}) d^\dagger_\sigma(\mathbf{k}) d_\sigma(\mathbf{k}) + V\sum_i c^\dagger_i d_i + \text{H.c.} + J_K \vec{S}^s_i \cdot \vec{S}^{Nd}_i, \tag{11}$$

where $d^\dagger_i$ creates a hole for the Nd orbital. Note here $c^\dagger_i$ creates the spin-one doublon and thus is different from the model in Ref. [7]. If the density of Nd holes is $n_{Nd} = 1 - \delta$, then the density for spin-one holes is $n_c = x + \delta$. In principle δ can have both doping and temperature dependence. Especially, δ is expected to decrease when we increase x [5]. One can see that $n_c = \delta \neq 0$ even for $x = 0$ if there is electron pocket from

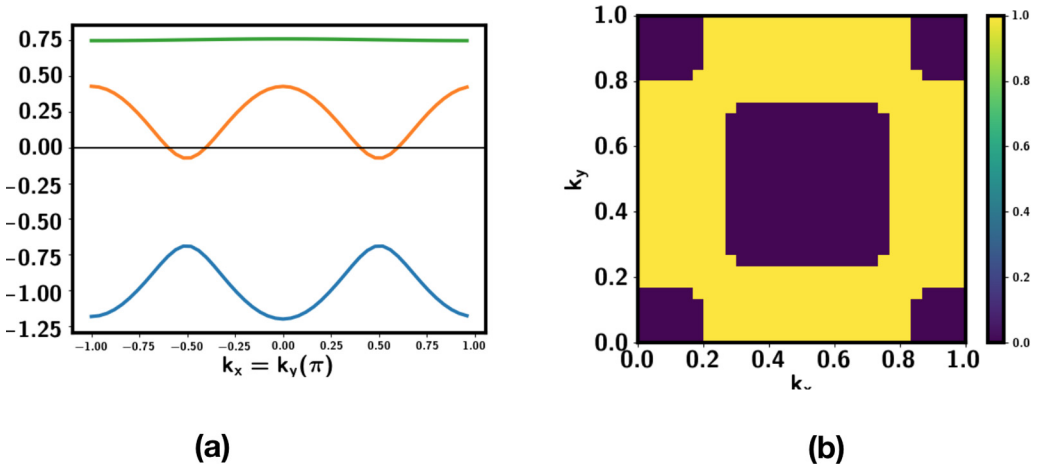

FIG. 2. Band structure at $x = 20\%$ in terms of $\psi_{i;2\sigma}$, $\tilde{f}_{i;\sigma} = f^\dagger_{i;\sigma}$, and $\tilde{\psi}_{i;1\sigma} = \psi^\dagger_{i;1\sigma}$. We use $t = 2J$ and $J' = 4J$. The pairing term is suppressed by hand. For this specific choice of parameters, the resulting $n(\mathbf{k})$ in (b) shows two electron pockets.

Nd in the Fermi level. This self-doping effect can explain why the undoped compound is metallic and does not have magnetic order.

VI. CONCLUSION

In summary, we propose a t-J model with spin-one hole (doublon in hole picture) to model the hole-doped $NdNiO_2$. We introduce two distinct parton theories to analyze this unconventional model. Specifically, we find that a Fermi liquid or d-wave superconductor is possible in this model, arising from the Kondo resonance between the spin-one doublon and spin-1/2 singly occupied state. This suggests that a combination of heavy fermion physics and cuprate physics may emerge in this model. We hope the proposed model and the parton framework introduced in this paper will motivate further theoretical and numerical studies, as well as experiments probing the spin-orbital nature of doped holes in this superconductor.

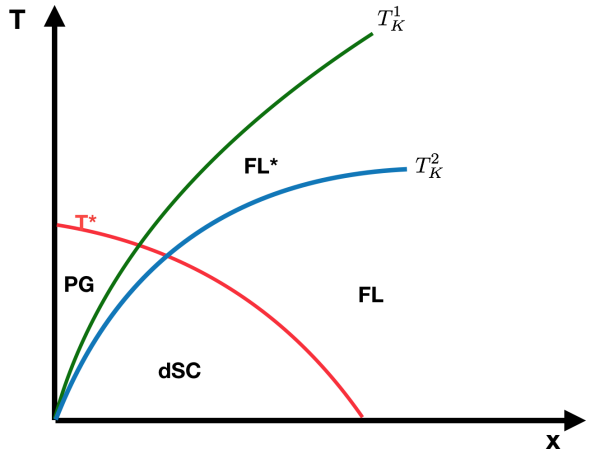

FIG. 3. Sketch of phase diagram in the $T - x$ space extrapolating from the zero-temperature mean-field theory. There are two "Kondo" scales: T_K^1 and T_K^2. T_K^1 is associated with $\Delta_{f\psi_2}$. T_K^2 is associated with Φ_2. T^* determines the onset of Δ_f.

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APPENDIX A: MICROSCOPIC DERIVATION OF t-J MODEL WITH SPIN-ONE DOUBLON

1. Distinction from cuprates: Spin-one hole

Because the oxygen p orbital is far away from Fermi level in $NdNiO_2$, the doped hole will enter the d orbitals. From the LDA + U calculation [5,7], the energy splitting of the two e_g orbitals is 0.7 eV and smaller than the interaction scale. Therefore we need to include both $d_{x^2-y^2}$ and d_{z^2} orbitals. We choose to study the following model in the hole picture:

$$H = H_K + \frac{U_1}{2}\sum_i n_{1;i}(n_{1;i}-1) + \frac{U_2}{2}\sum_i n_{2;i}(n_{2;i}-1) + U'\sum_i n_{1;i}n_{2;i} - 2J_H\sum_i\left(\mathbf{S}_{1;i}\cdot\mathbf{S}_{2;i} + \frac{1}{4}n_{i;1}n_{i;2}\right), \tag{A1}$$

where $n_{a;i}$ is the density of orbital a at site i, $a = 1, 2$ denotes the $d_{x^2-y^2}$ and the d_{z^2} orbital, respectively, U_1, U_2 are the intraorbital Hubbard interaction, U' is the interorbital interaction, and J_H is the interorbital Hund's coupling. We expect $U_1 = U_2 = U$ and $U - U' = 2J_H$ [27].

The kinetic energy is

$$H_K = \sum_i \epsilon_{dd} n_{2;i} + \sum_{\langle ij\rangle} t_{1;ij} c^\dagger_{1;i} c_{1;j} + \sum_{\langle ij\rangle} t_{2;ij} c^\dagger_{2;i} c_{2;j} + \sum_{\langle ij\rangle} t_{12;ij} c^\dagger_{1;i} c_{2;j} + \text{H.c.}, \tag{A2}$$

where ϵ_{dd} is the splitting between the two e_g orbitals.

At zero doping, because $\epsilon_{dd} > 0$, the ground state has one hole on the $d_{x^2-y^2}$ orbital at each site. Next we discuss the fate of the doped hole. The energy cost for the hole to enter the orbital 1 is U_1, while the energy cost for the hole to be at orbital 2 is $\epsilon_{dd} + U' - J_H$. In the case that $\epsilon_{dd} < U - U' + J_H$, the orbital-singlet, spin-triplet configuration is energetically favored. In this paper we take $U = 3.4$ eV, $U' = 2$ eV [6], and $\epsilon_{dd} = J_H = 0.7$ eV [5,6]. We conclude that the doped hole in nickelate creates a spin-one d^8 site. Therefore the low-energy physics is governed by an unconventional t-J model with a spin-one hole.

2. t-J model

Next we drive the low-energy t-J model. First we need to define the Hilbert space.

Relation to the SU(4) symmetric model. The model in Eq. (A1) can be viewed as descending from a $SU(4)$ symmetric model but with anisotropies that lower the symmetry. At the $SU(4)$ symmetric point, at the filling $\nu_T = 1 + x$, the t-J model at the $U \gg t$ limit has a Hilbert space with dimension $10 = 4 + 6$ at each site. These 10 states can be divided to four singly occupied states and six doubly occupied states [25]. For simplicity, let us call them singlon and doublon. Singlon is in the fundamental representation of $SU(4)$, while the doublon is in the $SO(6)$ representation [25]. In the nickelates, anisotropies can further constrain the Hilbert space to be five dimensions at each site. There are three large anisotropies: ϵ_{dd}, $U - U'$, and J_H.

We note here that the relevant hopping t is entirely determined by t_2, the hopping between the d_{z^2} orbitals. The hopping within the $d_{x^2-y^2}$ is blocked since we have eliminated doublons living in a single orbital ($U' \ll U$ limit), and interorbital hopping is also eliminated for the same reason. We have not found an estimate for t_2, but we can estimate this to be of the order of $t_1 \sim 0.1$ eV [6]. Thus, we may assume we are in the $\epsilon_{dd} \gg t$, $U - U' \gg t$, and $J_H \gg t$ limit, where we can further restrict the doublon states by doing the $\frac{t}{U-U'}$ and $\frac{t}{J_H}$ expansion.

First, the e_g orbital splitting $\epsilon_{dd} \sim 0.7$ eV [5]. Therefore there are only two singlon states: $|1\uparrow\rangle$ and $|1\downarrow\rangle$. The $|2\sigma\rangle$ should not be included in the low-energy Hilbert space. However, it does appear when we consider the doublons. For the six doublon states, because of the large $U - U' \sim 1 - 2$ eV, we should only consider the four states $|1\sigma_1\rangle \otimes |2\sigma_2\rangle$. If $J_H << t$, all of these four doublon states should be kept and we have $2 + 4 = 6$ states at each site. However, in the opposite limit $J_H \gg t$ which we assume, we should only include three doublon states corresponding to the three spin triplets. Therefore in total we only have $2 + 3 = 5$ states at each site in the low-energy theory.

a. Labeling the Hilbert space

We focus on the $U, \epsilon_{dd}, U - U', J_H \gg t$ limit and project to the five states at each site. The Hilbert space at each site consists of a spin-1/2 singlon and a spin-one doublon. We label the singlon with $\sigma = \uparrow, \downarrow$ and label the doublon with $a = x, y, z$. In terms of a microscopic electron, $|\sigma\rangle = c^\dagger_{1\sigma}|0\rangle$ and

$$
\begin{aligned}
|x\rangle &= -\frac{1}{\sqrt{2}}(c^\dagger_{1\uparrow}c^\dagger_{2\uparrow} - c^\dagger_{1\downarrow}c^\dagger_{2\downarrow})\,|0\rangle\,,\\
|y\rangle &= \frac{i}{\sqrt{2}}(c^\dagger_{1\uparrow}c^\dagger_{2\uparrow} + c^\dagger_{1\downarrow}c^\dagger_{2\downarrow})\,|0\rangle\,,\\
|z\rangle &= \frac{1}{\sqrt{2}}(c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} + c^\dagger_{1\downarrow}c^\dagger_{2\uparrow})\,|0\rangle\,.
\end{aligned}
\tag{A3}
$$

We also define a density operator at each site: $n_i = \sum_a |a\rangle\langle a|$. n_i measures the number of doublons. In this restricted Hilbert space, the matrix elements of $c_{1\sigma}$ vanish, i.e., $c_{1\sigma} = 0$. Also, $c_{2\sigma}$ has the following matrix elements:

$$
\begin{aligned}
c_{i;2\uparrow} &= \prod_{j<i}(-1)^{n_j}\frac{1}{\sqrt{2}}\big(|\uparrow\rangle_i\langle x|_i - i\,|\uparrow\rangle\langle y|_i - |\downarrow\rangle_i\langle z|_i\big),\\
c_{i;2\downarrow} &= \prod_{j<i}(-1)^{n_j}\frac{1}{\sqrt{2}}\big(-|\downarrow\rangle_i\langle x|_i - i\,|\downarrow\rangle\langle y|_i - |\uparrow\rangle_i\langle z|_i\big),
\end{aligned}
\tag{A4}
$$

where $\prod_{j<i}(-1)^{n_j}$ is the Jordan-Wigner string to enforce fermionic statistics.

We can define the spin operator $\mathbf{S^s}$ for the spin-1/2 singlon and spin operator $\mathbf{S^d}$ for the spin-one doublon. It is easy to show that

$$
\begin{aligned}
S^s_a &= \frac{1}{2}\sum_{\sigma,\sigma'}\sigma^a_{\sigma,\sigma'}\,|\sigma\rangle\langle\sigma'|\,,\\
S^d_a &= -i\sum_{b,c}\epsilon_{abc}\,|b\rangle\langle c|\,,
\end{aligned}
\tag{A5}
$$

where the Pauli matrices σ and the antisymmetric tensor ϵ are used.

b. Hamiltonian

The t-J Hamiltonian can be written as

$$
H = t_2\sum_{ij} c^\dagger_{i;2\sigma}c_{j;2\sigma} + \text{H.c.} + H_J. \tag{A6}
$$

We need to emphasize that the Hamiltonian is defined in the restricted five-states Hilbert space. Therefore $c_{i;2\sigma}$ should not be confused with a conventional electron operator. In other words, $H_J = 0$ does not reduce the Hamiltonian to a free fermion model.

We should include superexchange terms involving virtual hopping, which leads to the following spin coupling:

$$
\begin{aligned}
H_J = J\sum_{\langle ij\rangle}\left(\vec{S}^s_i\cdot\vec{S}^s_j - \frac{1}{4}n^s_i n^s_j\right) + J_d\sum_{\langle ij\rangle}\left(\vec{S}^d_i\cdot\vec{S}^d_j - n^d_i n^d_j\right)\\
+\frac{1}{2}J'\sum_{\langle ij\rangle}\left[\left(\vec{S}^s_i\cdot\vec{S}^d_j - \frac{1}{2}n^s_i n^d_j\right) + \left(\vec{S}^d_i\cdot\vec{S}^s_j - \frac{1}{2}n^d_i n^s_j\right)\right],
\end{aligned}
\tag{A7}
$$

where s, d label the spin operator for the singlon and doublon. $n^s_i = 1 - n_i$ and $n^d_i = n_i$ are the density of singlon and doublon states.

The spin coupling parameters are obtained from standard second-order perturbation theory. We have

$J = 4\frac{t_1^2}{U}$, $J_d = \frac{t_1^2}{U} + \frac{t_2^2}{U} + 2\frac{t_{12}^2}{U}$. $J' = \frac{1}{2}(J_1 + J_2) + \frac{t_2^2}{2J_H} - t_{12}^2(\frac{1}{\epsilon_{dd}} - \frac{1}{\epsilon_{dd}+J_H})$, where $J_1 = 2(\frac{t_1^2}{U_1+U'} + \frac{t_1^2}{U_1-U'})$ and $J_2 = 2(\frac{t_{12}^2}{U_2+U'+\epsilon_{dd}} + \frac{t_{12}^2}{U_1-U'-\epsilon_{dd}})$. The J' term contains a contribution proportional to $\frac{t_2^2}{2J_H}$, which is from integrating the orbital-triplet, spin-singlet doublon. The final value of J' depends on the details of the material, but it is definitely reasonable to assume that $J' > J$. Actually, if we assume $U = 2U' = 4J_H$, $\epsilon_{dd} = J_H$, $t_1 = t_{12}$, and $t_2 = 0$ (t_2 should be smaller in the xy plane because it is associated with the d_{z^2} orbital), we find $J' \approx 1.3J$. In the following we view $\frac{J'}{J}$ as a phenomenological parameter. The J' term can be viewed as a Kondo coupling between the spin-1/2 singlon and spin-1 doublon. It can cause Kondo resonance between them.

APPENDIX B: HAMILTONIAN IN THE SPIN-ONE SLAVE BOSON AND THREE-FERMION PARTON THEORY

In the main text we introduced two different parton constructions: spin-one slave boson and a three-fermion parton. Here we show that there is a connection between these two parton theories. The three-fermion parton can be derived from the slave boson parton by further fractionalizing the spin-one slave boson to two spin-1/2 fermions:

$$\begin{aligned} b_x^\dagger &= -\frac{1}{\sqrt{2}}(\psi_{1\uparrow}^\dagger \psi_{2\uparrow}^\dagger - \psi_{1\downarrow}^\dagger \psi_{2\downarrow}^\dagger), \\ b_y^\dagger &= \frac{i}{\sqrt{2}}(\psi_{1\uparrow}^\dagger \psi_{2\uparrow}^\dagger + \psi_{1\downarrow}^\dagger \psi_{2\downarrow}^\dagger), \\ b_z^\dagger &= \frac{1}{\sqrt{2}}(\psi_{1\uparrow}^\dagger \psi_{2\downarrow}^\dagger + \psi_{1\downarrow}^\dagger \psi_{2\uparrow}^\dagger). \end{aligned} \tag{B1}$$

The physical hole operator can then be written as

$$\begin{aligned} c_\uparrow &= \frac{1}{\sqrt{2}} f_\uparrow^\dagger (b_x - i b_y) - \frac{1}{\sqrt{2}} f_\downarrow^\dagger b_z \\ &= f_\uparrow^\dagger \psi_{1\uparrow}\psi_{2\uparrow} + \frac{1}{2} f_\downarrow^\dagger (\psi_{1\uparrow}\psi_{2\downarrow} + \psi_{1\downarrow}\psi_{2\uparrow}), \\ c_\downarrow &= -\frac{1}{\sqrt{2}} f_\downarrow^\dagger (b_x + i b_y) - \frac{1}{\sqrt{2}} f_\uparrow^\dagger b_z \\ &= f_\downarrow^\dagger \psi_{1\downarrow}\psi_{2\downarrow} + \frac{1}{2} f_\uparrow^\dagger (\psi_{1\uparrow}\psi_{2\downarrow} + \psi_{1\downarrow}\psi_{2\uparrow}). \end{aligned} \tag{B2}$$

In terms of the slave boson construction, the hopping term in the t-J model can be rewritten as

$$\begin{aligned} H_K = &-\frac{t_2}{2}\sum_{\langle ij\rangle} f_{j\uparrow}^\dagger f_{i\uparrow}(b_{i;x}^\dagger b_{j;x} + b_{i;y}^\dagger b_{j;y} + b_{i;z}^\dagger b_{j;z}) \\ &- \frac{t_2}{2}\sum_{\langle ij\rangle} f_{j\downarrow}^\dagger f_{i\downarrow}(b_{i;x}^\dagger b_{j;x} + b_{i;y}^\dagger b_{j;y} + b_{i;z}^\dagger b_{j;z}) \\ &- t_2 \sum_{\langle ij\rangle}\sum_{a=x,y,z} (f_j^\dagger S_a^f f_i)(b_i^\dagger S_a^b b_j). \end{aligned} \tag{B3}$$

In terms of the three-fermion parton construction, the kinetic part is

$$\begin{aligned} H_K = &-\frac{1}{4}t_2 \sum_\sigma \sum_{\langle ij\rangle} f_{j\sigma}^\dagger f_{i\sigma}(\psi_{i;2\downarrow}^\dagger \psi_{i;1\uparrow}^\dagger + \psi_{i;2\uparrow}^\dagger \psi_{i;1\downarrow}^\dagger) \\ &\times (\psi_{j;1\uparrow}\psi_{j;2\downarrow} + \psi_{j;1\downarrow}\psi_{j;2\uparrow}) \\ &- t_2 \sum_\sigma \sum_{\langle ij\rangle} f_{j;\sigma}^\dagger f_{i;\sigma} \psi_{i;2\sigma}^\dagger \psi_{i;1\sigma}^\dagger \psi_{j;1\sigma}\psi_{j;2\sigma} \\ &-\frac{1}{2}t_2 \sum_{\langle ij\rangle} f_{j;\uparrow}^\dagger f_{i;\downarrow}[(\psi_{i;2\downarrow}^\dagger \psi_{i;1\uparrow}^\dagger + \psi_{i;2\uparrow}^\dagger \psi_{i;1\downarrow}^\dagger)(\psi_{j;1\uparrow}\psi_{j;2\uparrow}) \\ &+ (\psi_{i;2\downarrow}^\dagger \psi_{i;1\downarrow}^\dagger)(\psi_{j;1\uparrow}\psi_{j;2\downarrow} + \psi_{j;1\downarrow}\psi_{j;2\uparrow})] \\ &-\frac{1}{2}t_2 \sum_{\langle ij\rangle} f_{j;\downarrow}^\dagger f_{i;\uparrow}[(\psi_{i;2\downarrow}^\dagger \psi_{i;1\uparrow}^\dagger + \psi_{i;2\uparrow}^\dagger \psi_{i;1\downarrow}^\dagger)(\psi_{j;1\downarrow}\psi_{j;2\downarrow}) \\ &+ (\psi_{i;2\uparrow}^\dagger \psi_{i;1\uparrow}^\dagger)(\psi_{j;1\uparrow}\psi_{j;2\downarrow} + \psi_{j;1\downarrow}\psi_{j;2\uparrow})] + \text{H.c.} \end{aligned} \tag{B4}$$

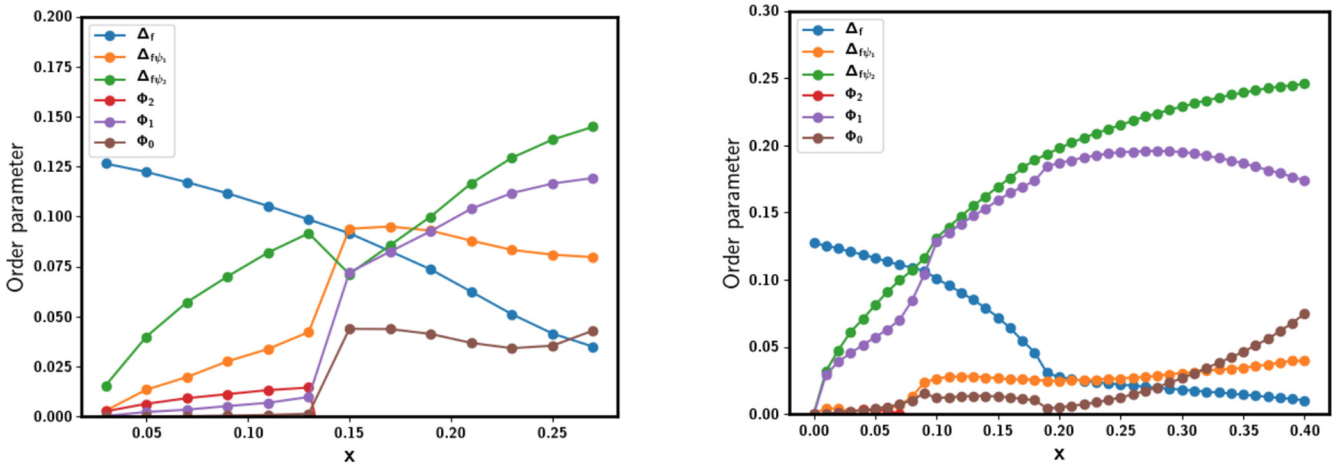
APPENDIX C: MEAN-FIELD THEORY AND SELF-CONSISTENT EQUATIONS

We list the mean-field theory from the three-fermion parton and self-consistent equations for a very general mean-field ansatz here. We include the spin-triplet pairing term of Ψ in the mean-field ansatz. Triplet pairing breaks the $SO(3)$ spin rotation, and we choose the pairing channel to be $\psi_{i;1\uparrow}\psi_{i;2\uparrow} - \psi_{i;1\downarrow}\psi_{i;2\downarrow}$. This pairing has the same spin rotation symmetry as $b_x^\dagger$.

We can have a mean-field theory by decoupling the original Hamiltonian:

$$\begin{aligned} H_M = &-t_f \sum_{\langle ij\rangle} f_{i\sigma}^\dagger f_{j\sigma} + \text{H.c.} - t_{ab}^\psi \sum_{ab=1,2}\sum_{\langle ij\rangle} \psi_{i;a}^\dagger \psi_{j;b} + \text{H.c.} \\ &- \Phi_a \sum_{\langle ij\rangle}(f_{i\sigma}^\dagger \psi_{j;a\sigma} + \psi_{i;a\sigma}^\dagger f_{j\sigma}) \\ &+ \text{H.c.} - \Phi_a^0 \sum_i (f_i^\dagger \psi_{i;a} + \psi_{i;a}^\dagger f_i) \\ &- \mu_f \sum_i n_i^f - \mu_1 \sum_i n_{i;1}^\psi - \mu_2 \sum_i n_{i;2}^\psi \\ &- \mu_x \sum_i (\psi_{i;1}^\dagger \psi_{i;2} + \text{H.c.}) \\ &+ \sum_{\langle ij\rangle} \Delta_{f;ij}(f_{i;\uparrow}^\dagger f_{j;\downarrow}^\dagger - f_{i\downarrow}^\dagger f_{j;\uparrow}^\dagger) + \text{H.c.} \\ &+ \sum_{\langle ij\rangle} \Delta_{f,\psi_a;ij}[(f_{i;\uparrow}^\dagger \psi_{j;a\downarrow}^\dagger - f_{i;\downarrow}^\dagger \psi_{j;a\uparrow}^\dagger) \\ &+ (\psi_{i;a\uparrow}^\dagger f_{j;\downarrow}^\dagger - \psi_{i;a\downarrow}^\dagger f_{j;\uparrow}^\dagger)] + \text{H.c.} \\ &+ \Delta_t \sum_i (\psi_{i;1\uparrow}^\dagger \psi_{i;2\uparrow}^\dagger + \psi_{i;1\downarrow}^\dagger \psi_{i;2\downarrow}^\dagger) + \text{H.c.} \end{aligned} \tag{C1}$$

μ, μ_1, μ_2 are introduced to fix the density $\langle n_f\rangle = 1 - x$ and $\langle n_{\psi_1}\rangle = \langle n_{\psi_2}\rangle = x$. Meanwhile we need μ_{12} and μ_{21} to fix the constraint that $\Psi_i^\dagger \tau_{x,y} \Psi_i = 0$.



(a) $t = 1.5J, J' = 3J$ **(b)** $t = 2J, J' = 4J$

FIG. 4. Order parameters from mean-field equations.

Although there is triplet pairing, there is still time-reversal symmetry. Therefore any correlation for spin up and spin down is guaranteed to be equal. This can greatly simplify our self-consistent equations.

Following the standard variational principle [28], self-consistent equations can be derived:

$$
\begin{aligned}
t^f &= \frac{3}{8}J\chi_f + \frac{3}{8}t(\chi_1\chi_2 - \chi_{21}\chi_{12}) + \frac{1}{4}t|\chi_{\Delta_t}|^2 \\
t_1^\psi &= \frac{3}{8}t\chi_f\chi_2 - \frac{9}{16}tC_{2j}C_{2i} \\
t_2^\psi &= \frac{3}{8}t\chi_f\chi_1 - \frac{9}{16}tC_{1j}C_{1i} \\
t_{12}^\psi &= -\frac{3}{8}t\chi_f\chi_{21} + \frac{9}{16}tC_1C_2 \\
\Delta_{ij} &= \frac{3}{8}J\chi_\Delta \\
\Delta_t &= -\frac{1}{2}t\chi_f\chi_{\Delta_t} \\
\Delta_{f\psi_a} &= \frac{3}{16}J'\chi_{\Delta_{f\psi_a}} \\
\Phi_a &= \frac{3}{16}J'C_a \\
\Phi_1^0 &= t\sum_{j\sim i}\left(-\frac{5}{8}C_1\chi_2 + \frac{5}{8}C_2\chi_{12}\right) \\
\Phi_2^0 &= t\sum_{j\sim i}\left(-\frac{5}{8}C_2\chi_1 + \frac{5}{8}C_1\chi_{12}\right),
\end{aligned}
\tag{C2}
$$

where

$$
\begin{aligned}
\chi_f &= \sum_\sigma \langle f_{j;\sigma}^\dagger f_{i;\sigma}\rangle \\
\chi_a^\psi &= \sum_\sigma \langle \psi_{j;a\sigma}^\dagger \psi_{i;a\sigma}\rangle \\
\chi_{12}^\psi &= \sum_\sigma \langle \psi_{j;1\sigma}^\dagger \psi_{i;2\sigma}\rangle \\
C_a^0 &= \sum_\sigma \langle \psi_{j;a\sigma}^\dagger f_{j;\sigma}\rangle \\
C_a &= \sum_\sigma \langle \psi_{j;a\sigma}^\dagger f_{i;\sigma}\rangle \\
\chi_\Delta &= \langle f_{i\uparrow}f_{j\downarrow} - f_{i\downarrow}f_{j\uparrow}\rangle \\
\chi_{\Delta_{f\psi_a}} &= \langle \psi_{i;a\uparrow}f_{j\downarrow} - \psi_{i;a\downarrow}f_{j\uparrow}\rangle \\
\chi_{\Delta_t} &= \langle \psi_{i;2\uparrow}\psi_{i;1\uparrow} + \psi_{i;2\downarrow}\psi_{i;1\downarrow}\rangle.
\end{aligned}
\tag{C3}
$$

The mean-field solutions are shown in Fig. 4. In our mean-field calculation, the Kondo couplings Φ_1 and $\Delta_{f\psi_2}$ decrease rapidly when decreasing J'. It is not clear whether this is an artifact of our naive mean-field treatment or not.

APPENDIX D: $J_H \to 0$ LIMIT: HEAVY FERMION PHYSICS

As we argued previously, a proper model for nickelate is a t-J model with a spin-one doublon, which is derived from $J_H \gg t$ limit. In this section we show that a heavy-fermion-like model can be written down at finite J_H. The model then reduces to the t-J model with a spin-one doublon if we take the $J_H \to \infty$ limit. As we will see later, this model at small J_H actually captures some of the essential physics connecting to the $J_H \gg t$ limit.

At finite J_H, we should keep $2 + 4 = 6$ states at each site. At each site the $6 = 2 \times 3$ dimensional Hilbert space has a tensor product structure: $H_i = H_i^1 \otimes H_i^2$, where H_i^a means the Hilbert space for orbital $a = 1, 2$ at site i. H_i^1 is a spin-1/2 on orbital one, and H_i^2 is a three-dimensional space generated by the hole operator $c_{2\sigma}^\dagger$ with the constraint $n_{i;2} = 0, 1$. Basically, the doped hole enters orbital 2 while the density on orbital 1 is fixed to be one per site. Therefore the final theory consists of xN_s $c_{2\sigma}$ particles moving and interacting with spin-1/2 moment at each site.

The final model is quite similar to a Kondo-Heisenberg lattice model:

$$H = t_2 \sum_{\langle ij\rangle} P c^\dagger_{i;2\sigma} c_{j;2\sigma} P + \text{H.c.} - \mu \sum_i c^\dagger_{i;2\sigma} c_{i;2\sigma} - 2J_H \sum_i \vec{S}^2_i \cdot \vec{S}^1_i + J \sum_{\langle ij\rangle} \vec{S}^1_i \cdot \vec{S}^1_j + \frac{1}{2}(J_1 - J) \sum_{\langle ij\rangle} [n_{i;2}(1-n_{j;2}) + (1-n_{i;2}) n_{j;2}] \vec{S}^1_i \cdot \vec{S}^1_j + \frac{1}{2} J_2 \sum_{\langle ij\rangle} \left(\vec{S}^1_i \cdot \vec{S}^2_j + \vec{S}^2_i \cdot \vec{S}^1_j \right) + J_d \sum_{\langle ij\rangle} \vec{S}^2_i \cdot \vec{S}^2_j, \quad \text{(D1)}$$

where J_1, J_2 is the spin coupling between the singlon and the spin of the doublon. The $(J_1 - J)$ term reflects the fact that the coupling between two nearest-neighbor spins on orbital 1 is different if one site is a singlon and the other one is a doublon. P constrains $n_{i;2} = 0, 1$. On average we have $\langle n_{i;2}\rangle = x$.

We have $J = 4\frac{t_1^2}{U_1}$, $J_d = 4\frac{t_2^2}{U_2}$. $J_1 = 2(\frac{t_1^2}{U_1+U'} + \frac{t_1^2}{U_1-U'})$ and $J_2 = 2(\frac{t_{12}^2}{U_2+U'+\epsilon_{dd}} + \frac{t_{12}^2}{U_1-U'-\epsilon_{dd}})$. Assuming $U_1 = U_2 = U$ and $U' = \frac{1}{2}U$ and $\epsilon_{dd} = \frac{1}{4}U$, we have $J_1 = \frac{4}{3}J$. If we further assume $t_{12} = t_1$, then $J_2 = \frac{4}{3}J$.

In the following we assume $J_1 = J$ for simplicity. Then the above model resembles the models for heavy fermion systems. Basically the particle on orbital 1 contributes a local spin-1/2 moment while orbital 2 provide itinerant particles. In this model, the itinerant electrons couple to the local moment through both ferromagnetic J_H and antiferromagnetic "Kondo" coupling. The model in Eq. (D1) reduces to the model in Eq. (4) if we take the $J_H \to \infty$ limit. (Interestingly, the $J_H \to -\infty$ limit gives the conventional t-J model in cuprate.)

When $J_H = 0$, itinerant holes from $c_{2\sigma}$ couple to the spin-1/2 moment. A "heavy Fermi liquid" or heavy fermion superconductor may show up through Kondo resonance. However, the large J_H limit is not clear at all from the above Hamiltonian. With a large J_H, $c_{2\sigma}$ itself cannot move coherently because it strongly couples to the spin-1/2 at the same site. Then the t-J model in Eq. (4) may be a better starting point. However, as we show in the main text, even in the $J_H \to \infty$ limit, a similar heavy fermion physical may emerge in the low energy. But there the small hole pocket is formed by fermion $\psi_{2\sigma}$ below T_K^1 (see Fig. 3), which is not identical to the microscopic $c_{2\sigma}$. We may view this $\psi_{2\sigma}$ operator as a "renormalized" operator in the infrared limit of RG flow. Our mean-field theory of the t-J model in the $J_H \to \infty$ limit shows that this renormalized hole $\psi_{2\sigma}$ can move coherently and does not feel frustration from J_H (after all, J_H disappears in the t-J model). Depending on whether there is Kondo resonance between $\psi_{2\sigma}$ and the spin-1/2 moment, we have a Fermi liquid with a large Fermi surface (or superconductor) or a fractionalized Fermi liquid (FL*) phase.

APPENDIX E: DIFFERENT PHASES IN THE THREE-FERMION PARTON THEORY

We discuss different phases described by the mean-field theory in Eq. (C1) in the three-fermion parton theory. For simplicity, we focus on the ansatz with $\Delta_f = 0$. The pairing term can be added later. Our parton construction has a $U(1) \times SU(2)$ gauge invariance. We can always choose a $SU(2)$ gauge to remove the $f_i^\dagger \psi_{i;2}$ term. We can have different phases corresponding to the remaining gauge structure [invariant gauge group (IGG)].

1. $U(1) \times SU(2)$: Kondo breakdown

If $\Phi_1^0 = \Phi_1 = \Phi_2 = \Delta_{f\psi_a} = 0$ and $t_1^\psi = t_2^\psi$, $t_{12}^\psi = 0$, our mean-field ansatz still has the full $U(1) \times SU(2)$ structure. In this case f and ψ are decoupled. From the decoupling of H_K, ψ can get both a hopping and triplet-pairing term. Let us forget the triplet-pairing term first. Then ψ_1 and ψ_2 form two separate hole pockets, which couple to $U(1)$ gauge field a and $SU(2)$ gauge field α. $SU(2)$ gauge field always mediates attractive interaction in the orbital singlet, spin-triplet channel. Therefore we conclude that there is no stable phase with the IGG $U(1) \times SU(2)$. Ψ is always gapped out by a spin-triplet pairing term Δ_t, and then the $SU(2)$ gauge field is confined. In this case, the resulting phase is exactly the same as that accessed by condensing the spin-one slave boson in the previous section. Depending on the ansatz of f, we can have either a spin-nematic d-wave superconductor or spin-nematic Fermi liquid.

2. $U(1)_a \times U(1)_\alpha$: $U(1)$ pseudogap metal

In this IGG, we still need $\Phi_1^0 = \Phi_2 = \Phi_0 = \Delta_{f\psi_a} = 0$. However, we introduce $t_1^\psi \neq t_2^\psi$ to Higgs $SU(2)$ to $U(1)$. $U(1)$ is generated by τ_z, and let us label it as α. Meanwhile, there is another $U(1)$ gauge field a shared by f and Ψ. They have the following charge: f couples to a, ψ_1 couples to $\frac{1}{2}A + \frac{1}{2}a + \frac{1}{2}\alpha$, and ψ_2 couples to $\frac{1}{2}A + \frac{1}{2}a - \frac{1}{2}\alpha$.

If $\Delta_f = 0$, we have a large Fermi surface from f and two smaller Fermi surfaces from ψ. This is a very exotic metal similar to the "deconfined metal" proposed in Ref. [25] for the $SU(4)$ model.

If $\Delta_f \neq 0$, a is Higgsed down to Z_2 and we can ignore it. We still have two small Fermi surfaces formed by ψ_1 and ψ_2. Meanwhile ψ_1 couples to $\frac{1}{2}A + \frac{1}{2}\alpha$ while ψ_2 couples to $\frac{1}{2}A - \frac{1}{2}\alpha$. Because f forms d-wave pairing, the physical electron must have an antinode gap. Around node $(\frac{\pi}{2}, \frac{\pi}{2})$ there should still be gapless excitations from convolution of f, ψ_1, ψ_2. We dub this phase a "$U(1)$ pseudogap metal" because of its similarity to the pseudogap metal in cuprates and a deconfined $U(1)$ gauge field.

3. $U(1)_a$: Deconfined metal and Z_4 pseudogap metal

We assume ansatz $t_1^\psi \neq t_2^\psi$ and $t_{12}^\psi \neq 0$ for Ψ, which fully Higgses the $SU(2)$ gauge field. Besides we need $\Phi_0 = \Phi_1 = \Phi_2 = \Delta_{f\psi_a} = 0$. Then we only have a $U(1)$ gauge field a. In this case, we have two sets of Fermi surfaces formed by f and $\psi_{1,2}$. The low-energy theory looks like

$$L = L_{FS}[f, 2a] + L_{FS}\left[\psi, \frac{1}{2}A + a\right]. \quad \text{(E1)}$$

We call this phase as a "deconfined metal" because of a deconfined $U(1)$ gauge field. The areas of the two Fermi surfaces are $1-x$ and x, respectively. They are strongly coupled together by gauge field a.

When there is also pairing for f: $\Delta_f \neq 0$, which Higgses a down to Z_4, we get a "pseudogap metal." But in this case the Fermi surface formed by ψ only couples to a Z_4 gauge field. There may be one or two hole pockets depending on details of hopping terms in ψ. But generically this is a stable metallic phase. Its property is similar to "orthogonal metal" [29], except that now the Z_4 gauge theory part also contains a gapless nodal fermion from f.

This "pseudogap phase" has the following properties: (1) The thermodynamic properties and transport properties are the same as Fermi liquid with small hole pockets. The size of the hole pocket is equal to $2x$. But the physical charge carried by ψ is only $1/2$. Therefore Hall number is x. (2) Green function of c is a convolution of f, ψ_1, ψ_2. f only has gapless excitation around $(\frac{\pi}{2}, \frac{\pi}{2})$. ψ_1, ψ_2 is likely to have pockets at either (0,0) or (π, π). The spectral function of the physical electron operator must only have gapless weights at around $(\frac{\pi}{2}, \frac{\pi}{2})$ after convolution. Both of these features resemble the pseudogap metal in hole-doped cuprate.

4. $U(1)_\alpha$: FL*

We add $\Phi_1 \neq 0$, which hybridizes f and ψ_1, but still assumes $\Phi_2 = \Phi_0 = 0$ and $t_{12}^{\psi} = 0$. Therefore ψ_2 is decoupled from f, ψ_1.

f couples to $2a$. ψ_1 couples to $\frac{1}{2}A + a + \frac{1}{2}\alpha$. ψ_2 couples to $\frac{1}{2}A + a - \frac{1}{2}\alpha$. After $\Phi \neq 0$, we have $a = \frac{1}{2}(A + \alpha)$. Therefore the final phase still has one deconfined $U(1)$ gauge field.

There are two sets of Fermi surfaces in the low energy. The first one is formed by f, ψ_1 and it couples to $A + \alpha$. The other one is formed by ψ_2 and it couples to A. We have $c \sim f^\dagger \psi_1 \psi_2$. After adding $f^\dagger \psi_1$, ψ_2 is the same as a physical electron. We can always redefine $\tilde{\alpha} = A + \alpha$. The final theory is

$$L = L_{FS}[f, \tilde{\alpha}] + L_{FS}[\psi_2, A]. \tag{E2}$$

This describes a FL* phase. Basically the Fermi liquid part from ψ_2 coexists with a neutral Fermi surface formed by f, ψ_1. Because there is no coupling like $\psi_1^\dagger \psi_2$, the two Fermi surfaces do not merge. Our constraint is $n_{\psi_1} = n_{\psi_2} = x$ and $n_f = 1 - x$. Thus the Fermi surface area of the Fermi liquid part is fixed to be x. Naively, f forms a $U(1)$ spin liquid with spinon Fermi surface and the Fermi surface area is $1/2$. In practice the spin liquid part may likely be confined. Then the phase is just a small hole pocket decoupled from the spin-$1/2$ moment. It is exactly the "small Fermi surface" phase above the Kondo scale we described in the $J_H = 0$ limit.

Next we add pairing Δ_f to the mean-field ansatz. The neutral part becomes a Z_2 Dirac spin liquid, and we still call the resulting phase FL*.

5. Fully Higgsed: Conventional Fermi liquid with large Fermi surface

Consider ansatz with $\Phi_0 \neq 0$ and $\Delta_{f\psi_2} \neq 0$. All of gauge fields are fully Higgsed. We finally have a conventional Fermi liquid. The Fermi surface area is decided by $n_f + n_1 + n_2 = 1 + x$, consistent with the Luttinger theorem. If we further introduce pairing, we get a conventional superconductor.

APPENDIX F: ROLE OF Nd ORBITALS

Here we comment on the possible role of $5d$ orbitals of the Nd element. Reference [7] suggests that the Nd orbital couples to the $d_{x^2-y^2}$ orbital of N_i like in the Anderson model, which gives Kondo resonance. At zero doping, there is indeed fluctuation between the d^9 state and d^8R state, where R denotes the Nd orbital. However, as we argued previously, the lowest energy of the d^8 state of Ni is a spin triplet occupying both e_g orbitals. Thus a more appropriate lattice model should involve both e_g orbitals of Ni, and the dominant process is to create the spin-one d^8 state:

$$\begin{aligned} H = &\sum_k \epsilon_k^1 c_1^\dagger(\mathbf{k}) c_1(\mathbf{k}) + \sum_k (\epsilon_k^2 + \epsilon_{dd}) c_2^\dagger(\mathbf{k}) c_2(\mathbf{k}) \\ &+ \sum_{\mathbf{k}} \epsilon^d(\mathbf{k}) d^\dagger(\mathbf{k}) d(\mathbf{k}) + V_1 \sum_i c_{i;1}^\dagger d_i + \\ &+ V_2 \sum_i c_{i;2}^\dagger d_i + \text{H.c} \\ &+ \frac{U_1}{2} \sum_i n_{1;i}(n_{1;i} - 1) + \frac{U_2}{2} \sum_i n_{2;i}(n_{2;i} - 1) \\ &+ U' \sum_i n_{1;i} n_{2;i} - 2J_H \sum_i (\mathbf{S}_{1;i} \cdot \mathbf{S}_{2;i} + \frac{1}{4} n_{i;1} n_{i;2}), \end{aligned} \tag{F1}$$

where d is the hole operator for the orbital of the Nd element. c_1, c_2 represents the hole operators for the two e_g orbitals of Ni.

Unlike the model in Ref. [7], the above model is not a simple Anderson model because of inclusion of the V_2 process. In the limit $J_H, U', U \gg V_1, V_2$, a Kondo spin coupling between the N_i and Nd spin can be derived from second-order perturbation:

$$H_{\text{kondo}} = \tilde{J} \sum_i \vec{S}_i^{N_i} \cdot \vec{S}_i^{\text{Nd}}, \tag{F2}$$

where

$$\tilde{J} = \frac{2V_1^2}{U_1} - 2V_2^2 \left(\frac{1}{U' - J_H} - \frac{1}{U'} \right). \tag{F3}$$

The superexchange involving V_2 actually induces a ferromagnetic Kondo coupling because of the Hund's coupling. From DFT calculation, V_1 is very tiny [7,8]. Reference [7] estimates $V_1 \approx 0.1 t_1$, which means $\tilde{J} \sim 0.01J$. Hence the Kondo coupling between the Nd and Ni can be ignored.

We always have the constraint $n_{N_i} + n_{\text{Nd}} = 1$. Once there are electrons in the Nd orbital, the N_i site is self-doped. In this case, we should expect a small doping x even for undoped $NdNiO_2$, and the physics should be mainly governed by the t-J model in Eq. (4) with small doping together with a small density of Nd electrons. This self-doping effect is likely to be the reason why the parent compound is metallic and does not have magnetic order. Besides, n_{Nd} can in principle vary with temperature. Decreasing of n_{Nd} below 60 K may be the reason why there is a change of the Hall coefficient for $x = 0.2$ and an upturn of resistivity for $x = 0$.

In the limit $U, U - U', \epsilon_{dd}, J_H \gg t$, we have a low-energy model which extends our t-J model:

$$H = H_{t\text{-}J} + \sum_k \xi_{\mathrm{Nd}}(\mathbf{k}) d_\sigma^\dagger(\mathbf{k}) d_\sigma(\mathbf{k}) + V \sum_i c_i^\dagger d_i + \mathrm{H.c.} + J_K \vec{S}_i^s \cdot \vec{S}_i^{\mathrm{Nd}}, \tag{F4}$$

where $d_i^\dagger$ creates a hole for the Nd orbital and $c_i^\dagger$ creates a spin-one doublon. We need to include J_K from V_1.

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