

Supplemental Material: Orbital-selective spin-triplet superconductivity in infinite-layer LaNiO_2

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I. DFT ELECTRONIC STRUCTURE

DFT calculations have been performed using the Vienna ab-initio Simulation Package (VASP) [1, 2], employing the projector augmented wave (PAW) method [3]. Exchange and correlation effects have been handled using the generalized gradient approximation (GGA) [4–6] within the Perdew-Burke-Ernzerhof (PBE) approach [7]. A plane-wave cutoff of 500 eV was used for the truncation of the basis set, while the relaxation of the electronic and ionic degrees of freedom was considered converged when the output difference between two steps was equal or smaller than 1×10^{-6} eV and 1×10^{-8} eV/Å, respectively. The chosen number of $\mathbf{k}$ -points is $16 \times 16 \times 16$. Partial occupancies have been determined via Gaussian smearing with a width of 0.1 eV. Spin-orbit coupling (SOC) has generally not been considered, unless stated otherwise, in which case SOC has been included self-consistently. The comparison between the cases with and without SOC is shown in Fig. S1(d). The SOC-induced shift in energy for a given band is typically on the order of 10 to 100 meV. Our calculations therefore indicate that the impact of SOC is negligible also in the renormalized regime.

In our DFT single-particle calculations, the paramagnetic phase of LaNiO_2 has been modeled by neglecting the spin-polarization degree of freedom. To justify this approach, and verify that the non-magnetic configuration accurately describes a paramagnetic state, we study several supercell configurations ($2 \times 2 \times 3$ expansions of the original unit cell) within the disordered local moment framework, i.e. assigning random magnetic moments to the Ni sites and ensuring that the total magnetic moment sums up to zero. This setup approximates the behavior of a real paramagnetic material. As shown in Fig. S2(b) to S2(f), the unfolded electronic band structures from several such magnetic configurations, subject to the constraints defined above, closely align with the results obtained from non-magnetic DFT calculations (Fig. S2(a)). This agreement supports the validity of the non-magnetic approximation for the paramagnetic state and its subsequent use in many-body analysis. For the purposes of the present work, the terms “non-magnetic” and “paramagnetic” can be considered as interchangeable and synonymous.

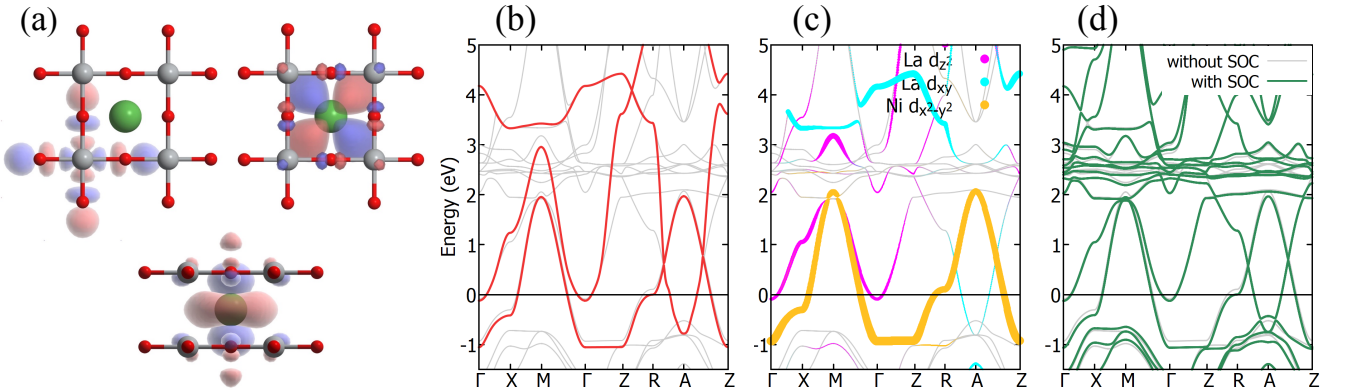


FIG. S1. (a) Isosurfaces of the Wannier orbitals used for the three-band model. The upper left and right panels show top views of the $\text{Ni } d_{x^2-y^2}$ and $\text{La } d_{xy}$ Wannier orbitals, respectively. The lower panel shows a side view of the $\text{La } d_{z^2}$ orbital. (b) Comparison between DFT band structure (gray lines) and bands derived from the three-band Wannier model (red lines). (c) DFT band structure projected onto the three orbitals of the model: $\text{La } d_{z^2}$, $\text{La } d_{xy}$, and $\text{Ni } d_{x^2-y^2}$. (d) Comparison between DFT band structures, with and without SOC.

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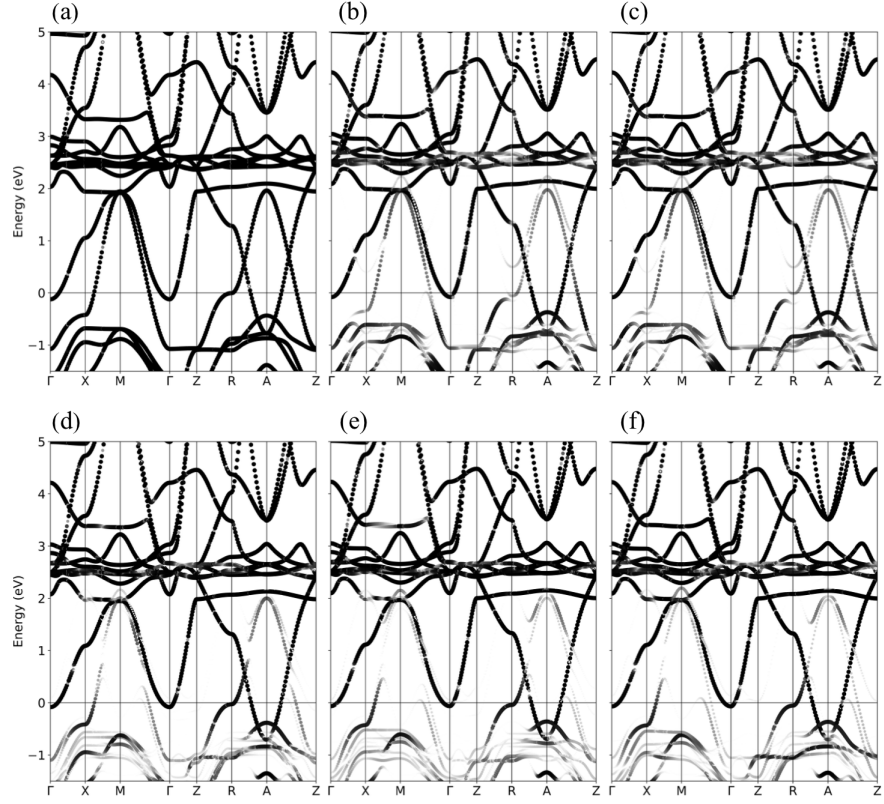


FIG. S2. Electronic band structures of LaNiO_2 at DFT level in several paramagnetic configurations. The weight of the dots represents the contribution of the supercell eigenstate in the primitive BZ. (a) Electronic structure of the pristine unit cell without magnetism. (b)–(f) Electronic structures of some magnetic supercells with average zero magnetization, unfolded in the primitive BZ.

Starting from the non-magnetic system and its corresponding electronic structure, Wannier functions [8, 9] have been used to provide an equivalent description of Bloch states via a maximally localized orbital basis. The Wannier-basis position matrix elements $\langle 0n|\hat{r}|Rm\rangle$, Rm being the maximally-localized Wannier function m in unit cell R , have been used for the tight-binding (TB) description, as shown in Figs. S1(a) and S1(b) [10–13]. For the three-band model, the projection functions used to build the initial guess $A(\mathbf{k})_{mn} = \langle \psi_{m\mathbf{k}}|g_n\rangle$ for the unitary transformation are provided by Ni $d_{x^2-y^2}$, La d_{xy} , and La d_{z^2} orbitals. $|g_n\rangle$ represents the trial localized orbitals, and $|\psi_{m\mathbf{k}}\rangle$ are the Bloch states. DFT band structures have been visualized using the VASPKIT postprocessing tool, as shown in Fig. S1(c) [14], while VESTA [15] has been used to visualize the Wannier-orbital isosurfaces and crystal structures in Fig. S1(a).

II. WANNIER HAMILTONIAN

We introduce the operator $\psi_\sigma^\dagger(\mathbf{k}) = [c_{1\sigma}^\dagger(\mathbf{k}), c_{2\sigma}^\dagger(\mathbf{k}), c_{3\sigma}^\dagger(\mathbf{k})]$ to describe the given multiband system. Here, $c_{l\sigma}^\dagger(\mathbf{k})$ is the fermionic creation operator, where σ and l denote the spin and orbital index, with $l = 1, 2, 3$ referring to the La $5d_{z^2}$, La $5d_{xy}$, and Ni $3d_{x^2-y^2}$ orbital, respectively. We thus write the non-interacting Hamiltonian as

$$H_0 = \sum_{\mathbf{k}\sigma} \psi_\sigma^\dagger(\mathbf{k}) h(\mathbf{k}) \psi_\sigma(\mathbf{k}). \quad (\text{S1})$$

For the derivation of the matrix elements in the Hamiltonian $h(\mathbf{k})$ we employ an energy cutoff of 0.01 eV for the TB hopping amplitudes. The Hamiltonian is given by

$$\begin{aligned} h_{11} &= \epsilon_1 - \mu + 2t_{11}^x (\cos k_x + \cos k_y) + 2t_{11}^{xx} (\cos 2k_x + \cos 2k_y) + 2t_{11}^z \cos k_z + 2t_{11}^{zz} \cos 2k_z \\ &\quad + 4t_{11}^{xzz} \cos 2k_z (\cos k_x + \cos k_y), \\ h_{22} &= \epsilon_2 - \mu + 2t_{22}^x (\cos k_x + \cos k_y) + 4t_{22}^{xy} \cos k_x \cos k_y + 2t_{22}^{xx} (\cos 2k_x + \cos 2k_y) \end{aligned} \quad (\text{S2})$$

$$\begin{aligned}
& + 4t_{22}^{xy}(\cos 2k_x \cos k_y + \cos k_x \cos 2k_y) + 2t_{22}^z \cos k_z + 2t_{22}^{zz} \cos 2k_z \\
& + 4t_{22}^{xz} \cos k_z (\cos k_x + \cos k_y) + 8t_{22}^{xyz} \cos k_x \cos k_y \cos k_z + 4t_{22}^{xzz} \cos k_z (\cos 2k_x + \cos 2k_y) \\
& + 8t_{22}^{xyx} \cos k_z (\cos 2k_x \cos k_y + \cos k_x \cos 2k_y) + 2t_{22}^{zzz} \cos 3k_z \\
& + 4t_{22}^{zzz} \cos 2k_z (\cos k_x + \cos k_y) + 4t_{22}^{xzzz} \cos 2k_z (\cos 2k_x + \cos 2k_y) \\
& + 8t_{22}^{xyzz} \cos 2k_z (\cos 2k_x \cos k_y + \cos k_x \cos 2k_y),
\end{aligned} \tag{S3}$$

$$\begin{aligned}
h_{33} = & \epsilon_3 - \mu + 2t_{33}^x (\cos k_x + \cos k_y) + 4t_{33}^{xy} \cos k_x \cos k_y + 2t_{33}^{xx} (\cos 2k_x + \cos 2k_y) + 2t_{33}^z \cos k_z \\
& + 8t_{33}^{xyz} \cos k_x \cos k_y \cos k_z,
\end{aligned} \tag{S4}$$

$$h_{12} = -4t_{12}^{xy} \sin k_x \sin k_y - 8t_{12}^{xyz} \sin k_x \sin k_y \cos k_z - 8t_{12}^{xyzz} \sin k_x \sin k_y \cos 2k_z, \tag{S5}$$

$$\begin{aligned}
h_{13} = & 8t_{13}^x (\cos 3/2k_x \cos 1/2k_y - \cos 1/2k_x \cos 3/2k_y) \cos 1/2k_z \\
& + 8t_{13}^{xz} (\cos 3/2k_x \cos 1/2k_y - \cos 1/2k_x \cos 3/2k_y) \cos 3/2k_z,
\end{aligned} \tag{S6}$$

$$\begin{aligned}
h_{23} = & -8t_{23}^x (\sin 3/2k_x \sin 1/2k_y - \sin 1/2k_x \sin 3/2k_y) \cos 1/2k_z \\
& - 8t_{23}^{xz} (\sin 3/2k_x \sin 1/2k_y - \sin 1/2k_x \sin 3/2k_y) \cos 3/2k_z.
\end{aligned} \tag{S7}$$

We use a chemical potential of $\mu = 9.28$ eV and $\mu = 9.12$ eV in the undoped and doped scenario, respectively. The corresponding TB parameters specified in units of eV are

$$\epsilon_1 = 12.3837, \epsilon_2 = 12.3325, \epsilon_3 = 9.6706, \tag{S8}$$

$$t_{11}^x = -0.4266, t_{11}^{xx} = 0.0401, t_{11}^z = -1.0314, t_{11}^{zz} = 0.1150, t_{11}^{xzz} = 0.0155, \tag{S9}$$

$$t_{22}^x = 0.3964, t_{22}^{xy} = -0.0602, t_{22}^{xx} = 0.0417, t_{22}^z = 0.3545, t_{22}^{zz} = -0.1680, t_{22}^{xyz} = 0.0571,$$

$$\begin{aligned}
t_{22}^{zz} = & -0.0549, t_{22}^{xzz} = -0.0242, t_{22}^{xyx} = -0.0230, t_{22}^{xyyz} = 0.0210, t_{22}^{zzz} = 0.0113, \\
t_{22}^{xzz} = & 0.0144, t_{22}^{xzzz} = 0.0103, t_{22}^{xyzz} = -0.0107,
\end{aligned} \tag{S10}$$

$$t_{33}^x = -0.3656, t_{33}^{xy} = 0.0941, t_{33}^{xx} = -0.0441, t_{33}^z = -0.0413, t_{33}^{xyz} = 0.0121, \tag{S11}$$

$$t_{12}^{xy} = 0.0777, t_{12}^{xyz} = -0.0541, t_{12}^{xyzz} = 0.0100, \tag{S12}$$

$$t_{13}^x = 0.0277, t_{13}^{xz} = -0.0142, \tag{S13}$$

$$t_{23}^x = -0.0183, t_{23}^{xz} = 0.0198. \tag{S14}$$

The density of states (DOS) of the unrenormalized system can be obtained from

$$\rho(\omega_n) = -\frac{1}{N\pi} \sum_k \text{Im Tr}[(i\omega_n \mathbb{1} - h(\mathbf{k}))^{-1}]. \tag{S15}$$

III. RENORMALIZED SUSCEPTIBILITIES AND SUPERCONDUCTING PAIRING

Within the orbital selective ansatz [16, 17], quasiparticles in orbital l are weighted by a factor $\sqrt{Z_l}$, i.e., $c_l^\dagger(\mathbf{k}) \rightarrow \sqrt{Z_l} c_l^\dagger(\mathbf{k})$, such that the Green's function in the orbital basis $G_{ll'}(\mathbf{k}, \omega_n)$ becomes

$$\tilde{G}_{ll'}(\mathbf{k}, \omega_n) = \sqrt{Z_l Z_{l'}} \sum_\mu \frac{a_\mu^l(\mathbf{k}) a_\mu^{l'*}(\mathbf{k})}{i\omega_n - E_\mu(\mathbf{k})}, \tag{S16}$$

where $E_\mu(\mathbf{k})$ is the eigenenergy of band μ . The renormalized Green's function enters the bare (non-interacting) susceptibilities, which after performing Matsubara-frequency summation read as

$$\tilde{\chi}_{l_1 l_2 l_3 l_4}^0(\mathbf{q}, \omega) = -\frac{1}{N} \sum_{\mathbf{k}, \mu\nu} \tilde{\eta}_{\mu\nu}(\mathbf{k}, \mathbf{q}) \frac{n_F(E_\nu(\mathbf{k} + \mathbf{q})) - n_F(E_\mu(\mathbf{k}))}{E_\nu(\mathbf{k} + \mathbf{q}) - E_\mu(\mathbf{k}) + \omega + i0^+}, \tag{S17}$$

with the Fermi-Dirac distribution n_F . Here, we have absorbed the quasiparticle weights into the dressing factor

$$\tilde{\eta}_{\mu\nu}(\mathbf{k}, \mathbf{q}) = \sqrt{Z_{l_1} Z_{l_2} Z_{l_3} Z_{l_4}} a_\mu^{l_4}(\mathbf{k}) a_\mu^{l_2*}(\mathbf{k}) a_\nu^{l_1}(\mathbf{k} + \mathbf{q}) a_\nu^{l_3*}(\mathbf{k} + \mathbf{q}), \tag{S18}$$

and $a_\mu^l(\mathbf{k})$ is the matrix element of the unitary transformation that connects band μ to orbital l . The homogeneous or physical bare spin susceptibility can be calculated by performing the sum

$$\tilde{\chi}_{\text{phys}}^0(\mathbf{q}) = \frac{1}{2} \sum_{ll'} \tilde{\chi}_{ll' l' l}^0(\mathbf{q}, 0) \tag{S19}$$

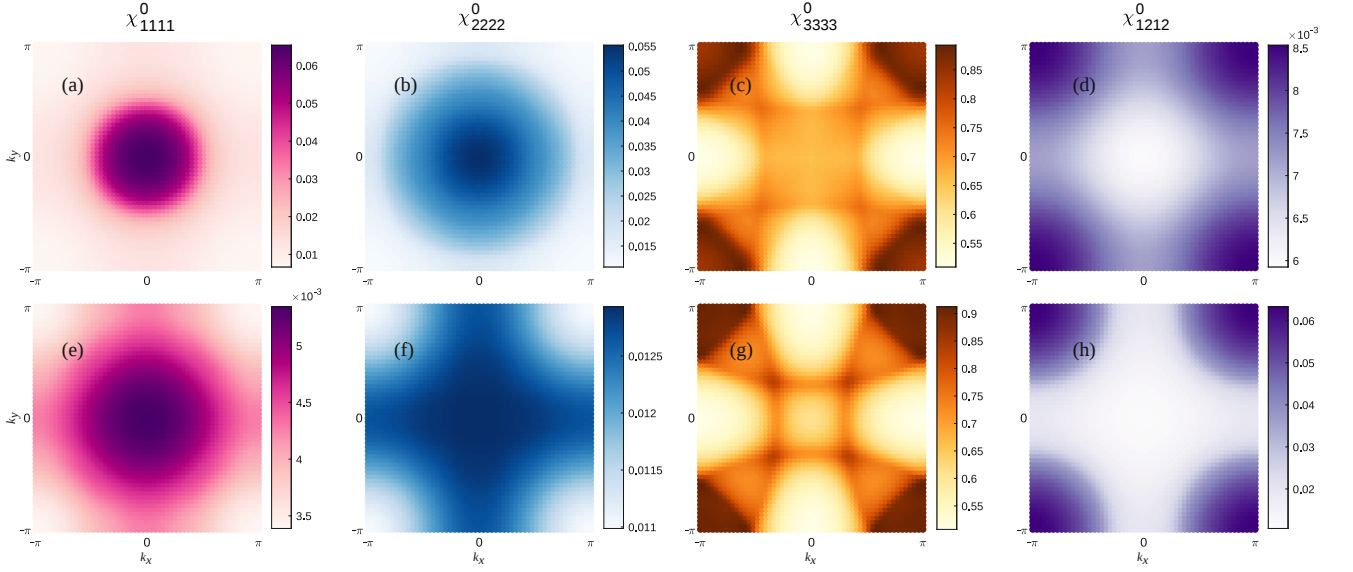


FIG. S3. Static ($\omega = 0$) bare susceptibilities of pristine LaNiO_2 for $Z_{d_{x^2-y^2}} = 1$ in the k_x k_y -plane for (a) - (d) $k_z = 0$ and (e) - (h) $k_z = \pi$. In panels (a), (e) $\tilde{\chi}_{1111}^0$, (b), (f) $\tilde{\chi}_{2222}^0$, and (c), (g) $\tilde{\chi}_{3333}^0$ represent the diagonal La d_{z^2} , La d_{xy} , and Ni $d_{x^2-y^2}$ orbital contributions, respectively. Moreover, we show the interorbital susceptibility $\tilde{\chi}_{1212}^0$ in panels (d) and (h). Momentum-space integration is done on a mesh of $60 \times 60 \times 60$ $\mathbf{k}$ -points.

of the static ($\omega = 0$) susceptibility [18]. In Fig. S3, we show plots of the bare susceptibilities $\tilde{\chi}_{1111}^0$, $\tilde{\chi}_{2222}^0$, $\tilde{\chi}_{3333}^0$, and $\tilde{\chi}_{1212}^0$ obtained for undoped LaNiO_2 without renormalization along 2D cuts ($k_z = 0, \pi$) through the Brillouin zone (BZ). Especially the $\tilde{\chi}_{3333}^0$ component shows nesting features familiar from the cuprates [19]. However, quasiparticle renormalization strongly dampens these features, such that they become less significant in the renormalized case. Note that for instance the interorbital susceptibility contribution $\tilde{\chi}_{1212}^0$ would not be observable within the physical susceptibility given in Eq. (S19).

Interactions are included in the calculation of susceptibilities within the random phase approximation (RPA). The spin-fluctuation and charge-fluctuation parts of the susceptibility are then given by [20]

$$\tilde{\chi}_{l_1 l_2 l_3 l_4}^{\text{RPA}, s}(\mathbf{q}, \omega) = \{\tilde{\chi}^0(\mathbf{q}, \omega)[\mathbb{1} - U^s \tilde{\chi}^0(\mathbf{q}, \omega)]\}_{l_1 l_2 l_3 l_4}^{-1}, \quad (\text{S20})$$

$$\tilde{\chi}_{l_1 l_2 l_3 l_4}^{\text{RPA}, c}(\mathbf{q}, \omega) = \{\tilde{\chi}^0(\mathbf{q}, \omega)[\mathbb{1} + U^c \tilde{\chi}^0(\mathbf{q}, \omega)]\}_{l_1 l_2 l_3 l_4}^{-1}. \quad (\text{S21})$$

In orbital space, the spin and charge interaction matrices U^s and U^c containing the interaction parameters are given by

$$U_{l_1 l_2 l_3 l_4}^s = \begin{cases} U_\tau, & l_1 = l_2 = l_3 = l_4, \\ U'_\tau, & l_1 = l_3 \neq l_2 = l_4, \\ J_\tau, & l_1 = l_2 \neq l_3 = l_4, \\ J'_\tau, & l_1 = l_4 \neq l_2 = l_3, \end{cases} \quad (\text{S22})$$

$$U_{l_1 l_2 l_3 l_4}^c = \begin{cases} U_\tau, & l_1 = l_2 = l_3 = l_4, \\ -U'_\tau + 2J_\tau, & l_1 = l_3 \neq l_2 = l_4, \\ 2U'_\tau - J_\tau, & l_1 = l_2 \neq l_3 = l_4, \\ J'_\tau, & l_1 = l_4 \neq l_2 = l_3, \end{cases} \quad (\text{S23})$$

respectively, where $\tau \in (\text{La}, \text{Ni})$ is the sublattice index.

In order to determine the superconducting (SC) pairing symmetries, we solve the linearized gap equation

$$\lambda_\alpha f_\alpha(\mathbf{k}) = \sum_j \oint_{C_j} \frac{d^2 k'_\parallel}{(2\pi)^2 v_F(\mathbf{k}')} \tilde{\Gamma}_{ij}(\mathbf{k}, \mathbf{k}') f_\alpha(\mathbf{k}'). \quad (\text{S24})$$

The largest eigenvalue λ_α of equation (S24) results in the highest transition temperature [18], while λ_α in general determines the pairing strength for the different pairing channels α [21]. The corresponding gap symmetries are identified by the eigenfunction $f_\alpha(\mathbf{k})$. The inverse of the Fermi velocity $v_F(\mathbf{k}) = |\nabla_{\mathbf{k}} E_\nu(\mathbf{k})|$ gives a measure of the DOS and momenta $\mathbf{k} \in C_i$, $\mathbf{k}' \in C_j$ are constrained to the FS sheets $C_{i,j}$. In Eq. (S24), $\tilde{\Gamma}_{ij}(\mathbf{k}, \mathbf{k}')$ represents the renormalized form of the effective multiorbital pair scattering vertex and is given by

$$\tilde{\Gamma}_{ij}(\mathbf{k}, \mathbf{k}') = \text{Re} \sum_{l_1 l_2 l_3 l_4} \sqrt{Z_{l_1}} \sqrt{Z_{l_4}} a_{\nu_i}^{l_1,*}(\mathbf{k}) a_{\nu_i}^{l_4,*}(-\mathbf{k}) \tilde{\Gamma}_{l_1 l_2 l_3 l_4}^{S/T}(\mathbf{k}, \mathbf{k}', \omega = 0) \sqrt{Z_{l_2}} \sqrt{Z_{l_3}} a_{\nu_j}^{l_2}(\mathbf{k}') a_{\nu_j}^{l_3}(-\mathbf{k}'), \quad (\text{S25})$$

$$\tilde{\Gamma}_{l_1 l_2 l_3 l_4}^S(\mathbf{k}, \mathbf{k}', \omega) = \left[\frac{3}{2} U^s \tilde{\chi}_{l_1 l_2 l_3 l_4}^{\text{RPA}, s}(\mathbf{k} - \mathbf{k}') U^s + \frac{1}{2} U^s - \frac{1}{2} U^c \tilde{\chi}_{l_1 l_2 l_3 l_4}^{\text{RPA}, c}(\mathbf{k} - \mathbf{k}') U^c + \frac{1}{2} U^c \right]_{l_1 l_2 l_3 l_4}, \quad (\text{S26})$$

$$\tilde{\Gamma}_{l_1 l_2 l_3 l_4}^T(\mathbf{k}, \mathbf{k}', \omega) = \left[-\frac{1}{2} U^s \tilde{\chi}_{l_1 l_2 l_3 l_4}^{\text{RPA}, s}(\mathbf{k} - \mathbf{k}') U^s + \frac{1}{2} U^s - \frac{1}{2} U^c \tilde{\chi}_{l_1 l_2 l_3 l_4}^{\text{RPA}, c}(\mathbf{k} - \mathbf{k}') U^c + \frac{1}{2} U^c \right]_{l_1 l_2 l_3 l_4}. \quad (\text{S27})$$

Here, $\tilde{\Gamma}_{l_1 l_2 l_3 l_4}$ determines the orbital vertex functions in the singlet (S) and triplet (T) channel. Physically, $\tilde{\Gamma}_{l_1 l_2 l_3 l_4}$ reflects particle-particle scattering of electrons from orbitals l_1, l_4 into orbitals l_2, l_3 . The quantities $U^s, U^c, \chi^{\text{RPA}}$ are matrices in orbital space and $\chi^{\text{RPA}, s/c}$ describes spin or charge fluctuations, respectively.

IV. STABILITY OF RPA ANALYSIS WITH RESPECT TO TB PARAMETERS

A recent debate regarding the pairing symmetry in the $\text{La}_3\text{Ni}_2\text{O}_7$ nickelate system [22, 23] stresses the importance of potential sensitivity of the RPA method to details of the input band structure and interaction parameters. In order to ensure the robustness of our results not just with respect to quasiparticle renormalization and interaction strength, which we discuss in the main text, we also investigate the impact of small modification to the TB model. When doing so, our aim is to keep the overall FS topology close to the one of the unchanged TB model. This results in a limitation of the variation of the hopping amplitudes. If, for instance, we vary the parameter t_{11}^z by $\pm 5\%$, the pocket around Γ notably changes in size, as can be seen in Fig. S4. For larger changes, it would eventually vanish or touch the $\text{Ni } 3d_{x^2-y^2}$ dominated surface, which represents a major deviation from the original fermiology. We take this as a point of reference and calculate the pairing symmetries for $\pm 5\%$ changes to the largest hopping amplitudes, i.e., $t_{11}^x, t_{11}^z, t_{22}^x, t_{22}^z$, and t_{33}^x .

As a result, we find that in all cases the leading renormalized solution still remains a degenerate (p_x, p_y) -wave state. In Table I, we list the corresponding ratio λ_T/λ_S of leading triplet over singlet eigenvalue for $U_{\text{La}}/U_{\text{Ni}} = 0.5$, $J_{\text{La}}/U_{\text{La}} = 0.2$, $U_{\text{Ni}} = 5 \text{ eV}$ and 20 eV , as well as $Z_{d_{x^2-y^2}} = 0.15$. Another modification that leaves the general FS topology intact would be given by alteration of the interorbital, i.e., hybridization terms in the Hamiltonian. Here, we checked the extreme case of essentially neglecting hybridization by setting all t_{12}, t_{13} , or t_{23} amplitudes to zero, both individually or together. Exemplary calculations with $J_{\text{La}}/U_{\text{La}} = 0.2$ and $U_{\text{Ni}} = 5 \text{ eV}$ show negligible changes of λ_T/λ_S , while confirming the degenerate p -wave solution. Hence, we conclude that our DFT band structure indeed permits a reliable RPA analysis and physically reasonable modifications to the TB model do not significantly alter the leading terms of the pairing symmetries.

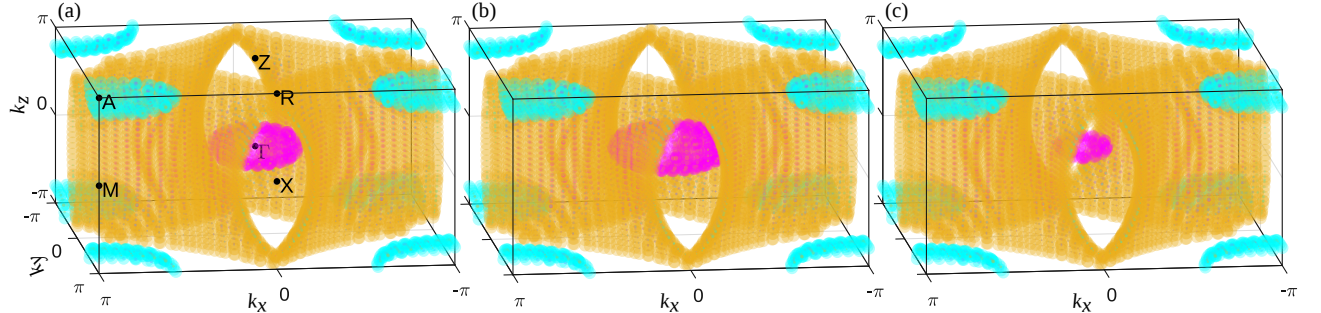


FIG. S4. 3D Fermi surfaces, with magenta, cyan, and yellow color referring to $\text{La } d_{z^2}$, $\text{La } d_{xy}$, and $\text{Ni } d_{x^2-y^2}$ orbital contributions, respectively. Shown are (a) the FS from the unchanged TB model, (b) the results from increasing t_{11}^z by 5%, and (c) from reducing t_{11}^z by 5%.

U_{Ni}	unchanged	$0.95 t_{11}^x$	$1.05 t_{11}^x$	$0.95 t_{11}^z$	$1.05 t_{11}^z$	$0.95 t_{22}^x$	$1.05 t_{22}^x$	$0.95 t_{22}^z$	$1.05 t_{22}^z$	$0.95 t_{33}^x$	$1.05 t_{33}^x$
5	3.67	3.16	3.73	2.95	3.69	3.47	3.30	3.90	3.44	3.71	3.56
20	2.53	1.85	3.96	1.75	4.81	2.48	2.41	2.55	2.47	2.48	2.50

TABLE I. Ratio λ_T/λ_S of the eigenvalues of the favored triplet and singlet channel for $U_{\text{La}}/U_{\text{Ni}} = 0.5$, $J_{\text{La}}/U_{\text{La}} = 0.2$, and $Z_{d_{x^2-y^2}} = 0.15$. The pairing symmetry remains E_u throughout.

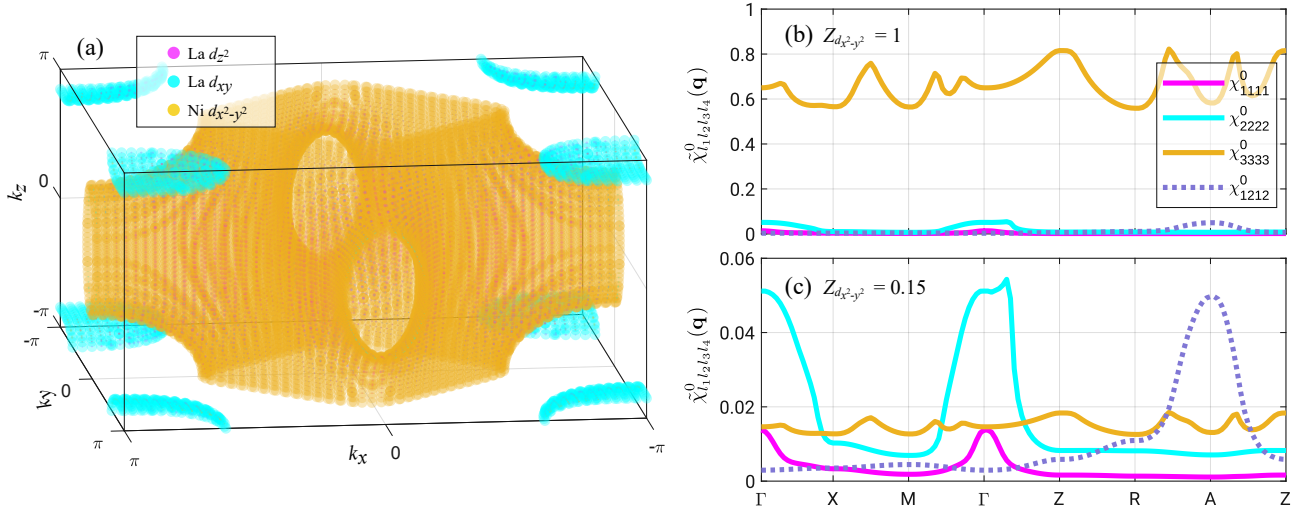


FIG. S5. (a) 3D Fermi surface including the orbital contributions relevant for the low-energy description of doped LaNiO_2 . Magenta, cyan, and yellow refer to the La d_{z^2} , La d_{xy} , and Ni $d_{x^2-y^2}$ orbitals, respectively. (b), (c) Static bare susceptibilities $\tilde{\chi}_{l_1 l_2 l_3 l_4}^0(\mathbf{q}, \omega = 0)$ for (b) $Z_{d_{x^2-y^2}} = 1$ and (c) $Z_{d_{x^2-y^2}} = 0.15$ for doped LaNiO_2 . The interorbital susceptibility $\tilde{\chi}_{1212}^0$ is shown in purple. The mesh for momentum space integration includes $80 \times 80 \times 80$ $\mathbf{k}$ -points.

V. DOPED LaNiO_2

Another natural question is whether the observed odd-parity p -wave state is also realized in doped LaNiO_2 . To investigate this, we capture the essential impact of doping by a rigid shift of the chemical potential, such that the Γ -centered electron pocket is lifted above the Fermi level. We show the corresponding 3D FS in Fig. S5(a). In the next step, we analyze the bare susceptibilities shown in Figs. S5(b) and S5(c). On the one hand, the diagonal susceptibility $\tilde{\chi}_{3333}^0$ loses its main peaks around the A and M points. On the other hand, once we introduce correlations by setting $Z_{d_{x^2-y^2}} = 0.15$, the central features are again given by the intraorbital rare-earth contributions $\tilde{\chi}_{1111}^0$ and $\tilde{\chi}_{2222}^0$ around Γ , as well as the interorbital component $\tilde{\chi}_{1212}^0$ around A. In contrast to undoped LaNiO_2 , the intraorbital La d_{xy} susceptibility $\tilde{\chi}_{2222}^0$ now far surpasses $\tilde{\chi}_{1111}^0$ from the La d_{z^2} orbital. This is not surprising since La d_{z^2} electrons used to contribute mainly to the pocket around Γ , which has vanished due to doping.

Finally, we also perform calculations of the pairing symmetry in doped LaNiO_2 , which can be seen in Fig. S6. Most interestingly, we observe that the essential conclusions made for the SC state of the undoped compound are still valid. The gap now clearly dominates on the remaining rare-earth pockets around A. In fact, the transition to a favored p -wave happens for even bigger quasiparticle weights of $Z_{d_{x^2-y^2}} \lesssim 0.3$, which might be facilitated due to a reduced DOS at the van Hove features around

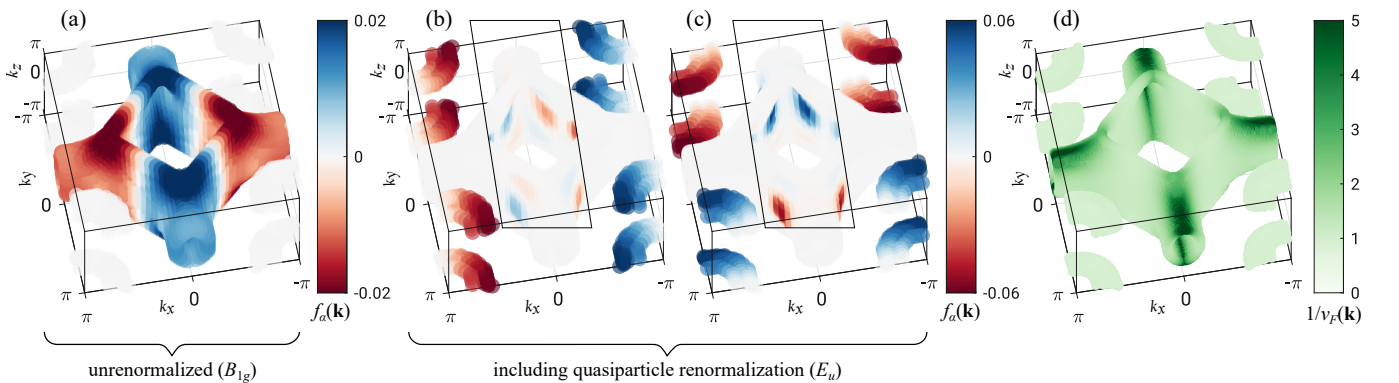


FIG. S6. Leading pairing structure of LaNiO_2 (a) without and (b), (c) with inclusion of quasiparticle renormalization. The gap symmetry changes from (a) an even-parity d -wave to (b), (c) a degenerate odd-parity p -wave solution. A color scale highlighting smaller amplitudes with maximum value of $\pm 1 \times 10^{-4}$ was chosen for the insets in panels (b), (c). (d) Inverse Fermi-velocity $1/v_F(\mathbf{k}) = 1/|\nabla_{\mathbf{k}} E_{\nu}(\mathbf{k})|$ giving a measure of the DOS. A total of 6800 points is taken for the 3D gap-structure calculations and we use $60 \times 60 \times 60$ $\mathbf{k}$ -points for momentum space integration.

R. For $Z_{d_{x^2-y^2}} = 0.15$, $U_{\text{La}}/U_{\text{Ni}} = 0.5$, $J_{\text{La}}/U_{\text{La}} = 0.2$ and $U_{\text{Ni}} = 5$ eV, the eigenvalue λ_T of the degenerate leading triplet solutions, i.e., their pairing strength, reaches $\lambda_T \approx 8.99\lambda_S$, with λ_S belonging to the leading singlet state. Intriguingly, this ratio is even greater than in pristine LaNiO_2 , where $\lambda_T \approx 3.67\lambda_S$ for the same set of parameters. However, note that doping reduces the effective-mass enhancement and thus could have a compensating effect.

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