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Published in:
Physical Review Letters

DOI:
10.1103/PhysRevLett.129.077002

Publication date:
2022

Document version
Publisher's PDF, also known as Version of record

Citation for published version (APA):
Kreisel, A., Andersen, B. M., Romer, A. T., Eremin, I. M., & Lechermann, F. (2022). Superconducting Instabilities in Strongly Correlated Infinite-Layer Nickelates. Physical Review Letters, 129(7), [077002]. https://doi.org/10.1103/PhysRevLett.129.077002
Superconducting Instabilities in Strongly Correlated Infinite-Layer Nickelates

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(Received 22 February 2022; accepted 19 July 2022; published 11 August 2022)

The discovery of superconductivity in infinite-layer nickelates has added a new family of materials to the fascinating growing class of unconventional superconductors. By incorporating the strongly correlated multiorbital nature of the low-energy electronic degrees of freedom, we compute the leading superconducting instability from magnetic fluctuations relevant for infinite-layer nickelates. Specifically, by properly including the doping dependence of the Ni $d_{\alpha\beta\gamma}$ and $d_{\alpha}$ orbitals as well as the self-doping band, we uncover a transition from $d$-wave pairing symmetry to nodal $s_\pm$ superconductivity, driven by strong fluctuations in the $d_{\alpha}$-dominated orbital states. We discuss the properties of the resulting superconducting condensates in light of recent tunneling and penetration depth experiments probing the detailed superconducting gap structure of these materials.

Calculations based on density functional theory (DFT) uncovered, besides a dominant Ni-$d_{\alpha\beta\gamma}$ dispersion, the importance of self-doping (SD) bands stemming from hybridizing Ni(3$d^\ell$) and rare-earth (5$d$) orbitals [18,22–24]. When including electronic correlations beyond DFT, the precise role of the Ni degrees of freedom and their mutual interplay with the SD character remain controversial. The main debate is between moderately to strongly correlated Ni-$d_{\alpha\beta\gamma}$-driven physics, and multiorbital Ni(3$d$) mechanisms [25,26]. In the former case, SC nickelates are described as cuprate-like with dominant $d_{\alpha\beta\gamma}$-wave SC pairing [22,27–33]. If additional SD-driven Kondo physics is taken into account, other intriguing $d$- and $s$-wave pairing solutions may become stabilized [34]. Furthermore, various multiorbital SC scenarios have been suggested [35,36], but in most cases those are based on rather simplified descriptions of the realistic correlated electronic structure. By contrast, approaching infinite-layer nickelates with a combination of DFT and dynamical-mean field theory (DMFT), including the effect of explicit Coulomb interactions on oxygen ions via self-interaction correction (SIC), in fact encourages the Ni multiorbital viewpoint for the normal state. In such DFT + SICDMFT calculations [18,37,38], the SC doping region is ruled by a strong interplay of Ni-$e_g$ $\{d_{\alpha\beta}\}$ degrees of freedom. Relevant Ni-$e_g$ physics is also suggested from Refs. [39,40].

Here, motivated by the recent experimental evidence against a simple SC $d_{\alpha\beta\gamma}$-wave scenario, we perform a detailed theoretical investigation of the leading pairing instabilities within a realistic multiorbital three-dimensional (3D) model for infinite-layer nickelates. The pairing kernel...
is generated by magnetic fluctuations, which are
constrained by recent resonant inelastic x-ray scattering
(RIXS) measurements mapping out dispersive magnetic
modes in these materials [41,42]. Intriguingly, the modifi-
cations of the electronic bands caused by doping naturally
induces a transition from d-wave order to s± SC. We
uncover the microscopic origin of this transition in the
leading pairing symmetry, and discuss consequences for
experiments probing the SC spectral gap.

Electronic model.—Treating correlation effects emerging
from the transition-metal (TM) and the ligand oxygen
sites on equal footing proves important for late TM oxides
with significant competition between Mott-Hubbard and
charge-transfer physics. As a result, the DFT + sicDMFT
approach [43] to infinite-layer nickelates, with their aniso-
tropic TM(3d)–O(2p) bonding situation due to the lack of
apical oxygen, gives rise to a dichotomic Mott-critical
regime of (nearly) insulating Ni–d⊥,y–y orbital and itinerant Ni–d⊥ orbital states.

This picture remains valid in a rotational-invariant slave-
boson [44,45] assessment of an effective three-band model,
tailored to reproduce the key DFT + sicDMFT findings at
stoichiometry [37]. The model hopping integrals \( t_{ij}^{ll} \) are
derived from a Wannier downfolding of the DFT band
structure, including Ni–d⊥, Ni–d⊥, and the SD band.
Supplemented with local Coulomb interactions, the effec-
tive Hamiltonian reads [37]

\[
H = \sum_{i,j,\ell,\ell'} \tilde{\epsilon}_{ij}^{l\ell} c_{i,\ell}^{\dagger}\sigma c_{j,\ell'}^{\sigma} + \sum_{i} \left[ H_{\text{int}}^{(i)} + H_{\text{orb}}^{(i)} \right]
\]

for \( \ell, \ell' = d, d_\perp, y \), SD and lattice sites \( i, j \). Note that
while the nearest-neighbor (NN) hopping between \( d \) and
SD is sizable with \( \sim 90 \) meV, it is absent between \( d_\perp \) and SD orbitals. Moreover, the in-plane NN hopping within
\( d_\perp \) is substantial with \( t_{c} \sim 390 \) meV, while within \( d \)
a comparable NN \( t_{c} \sim 400 \) meV along the \( c \) axis is active.
This highlights the competition of 2D vs 3D characteristics.

The on-site interaction part \( H_{\text{int}}^{(i)} \), notably only for the Ni–e_g
orbitals, has a two-orbital Slater-Kanamori form, i.e.,
includes density-density terms as well as pair-hopping
and spin-flip terms, and is parametrized by Hubbard \( U \)
and Hund’s coupling \( J \). The remaining noninteracting on-
site \( H_{\text{orb}}^{(i)} \) carries crystal-field terms via the on-site levels \( \epsilon_{\ell} \),
a double-counting correction in the fully localized-limit form [46] as well as a potential-shift term for the SD orbital.
The latter proves necessary to keep the SD band at the
stoichiometric Fermi level, in line with the DFT +
sicDMFT result [37]. The Eq. (1) model describes a (near)
orbital-selective Mott transition for \( d_\perp, y \) at \( U_c = 7 \) eV,
\( J = 1 \) eV. While the oxygen degrees of freedom are
integrated out, the model thus restores the DFT +
sicDMFT picture [18], since the realistic interplay of Ni-
and O-based correlations leads to the identical highly
correlated regime. The impact of the O-based correlations
is hence taken into account properly in the model, and
carried over to finite hole doping. The key correlation
effects from the slave-boson solution are then twofold:
renormalization of the dispersion via the quasiparticle (QP)
weights \( Z_{\ell}^{b} \) and renormalization of the effective on-site
levels via the shifts \( \Delta_{\ell} = \tilde{\epsilon}_{\ell} - \epsilon_{\ell} \) with \( \tilde{\epsilon}_{\ell} \) as the interacting
level energy. With doping, the nonzero quantities \( \Delta_{\ell} \) shift
the \( d_\perp \)-dominated flat band across the Fermi level, resulting
in an additional \( d_\perp \)-dominated Fermi-surface sheet (see Fig. 1). Both effects can be parametrized in a fully
renormalized band structure with the Hamiltonian

\[
H = \sum_{i,j,\ell,\ell'} \tilde{\epsilon}_{ij}^{l\ell} c_{i,\ell}^{\dagger}\sigma c_{j,\ell'}^{\sigma},
\]

with renormalized hoppings \( \tilde{\epsilon}_{ij}^{l\ell} \) taken from Ref. [37],
which is the basis of all further analysis in this Letter.

Magnetic fluctuations.—Intrinsic magnetism and sub-
stantial magnetic fluctuations have been recently revealed
by several experimental probes [15,41,47], and have also
been identified as important from first-principles calcula-
tions [38,48,49]. This motivates further theoretical studies of
these magnetic fluctuations themselves and their implication
for pairing. Specifically, RIXS measurements on the Ni L_23-
edge have uncovered a dispersive paramagnonlike mode
emanating from the \( \Gamma \) point with a bandwidth of approxi-
mately 200 meV; see Fig. 2 [41,47]. Starting from the slave-
boson solution to the effective Hamiltonian [Eq. (2)], we
follow the same procedure as in Refs. [50,51] to compute the
RIXS intensity. The RIXS process consists of a resonant
excitation of a Ni \( p \) state and a subsequent relaxation of a \( d \)
state together with the emission of a photon that is detected.

The calculation in second-order perturbation theory leads to
a sum of elements of the susceptibility tensor weighted with
the dipole matrix elements connecting Ni \( d \) and \( p \) states,
taking into account the polarization vectors of incoming and
outgoing x rays [51]. The matrix elements are obtained from
atomiclike orbitals and we calculate the bare susceptibility
structure of the SC gap function in systems prone to nickelates.\footnote{The method includes reduced pairing tendency from the most strongly correlated states, as these exhibit reduced QP weights at low energy. We stress that the self-consistently renormalized pair vertex is not incorporated, and the scheme merely mimics the effects of reduced orbital-dependent QP weights on the pairing structure.\footnote{This is also implied by the approximate renormalized interaction parameters in Eq. (2).}}

Approximating those weights by the diagonal part of the slave-boson QP-weight matrix, i.e., $Z_{\ell \ell'} = \delta_{\ell \ell'} Z_{\ell},$ the bare susceptibility acquires prefactors and reads $\sqrt{\sum_{\ell} Z_{\ell} Z_{\ell'} Z_{\ell} Z_{\ell'}}^{\ell} (q, \omega).$ Within random phase approximation this leads to the renormalized pairing interaction $\Gamma_{k,k'}$ when projected to the eigenstates at $k, k'$ on the FS.\footnote{The DFT + sicDMFT calculations\footnote{The DFT + sicDMFT calculations\footnote{This is also implied by the approximate renormalized interaction parameters in Eq. (2).}} deduced that the core of the $d_{x^2-y^2}$ and $d_{xy}$ orbitals have significant weight at low energies, and hence contribute to SC pairing.} The solution of the associated linearized gap equation,

$$- \frac{1}{V^2} \sum_{\eta} \int_{\mathbb{FS}} dS \Gamma_{k,k'} g_{l}(k') \frac{g_{l}(k)}{v_{F \mu}(k)} = \lambda_l g_{l}(k),$$

yields the gap symmetry function $g_{l}(k)$ of the instability $i$ with eigenvalue $\lambda_i.$\footnote{This is also implied by the approximate renormalized interaction parameters in Eq. (2).}

To illustrate this transition in the preferred pairing symmetry, we concentrate on the doping level $\delta = 0.16,$ and display in Fig. 3(a) the inverse Fermi velocity. It is

\begin{align}
\chi^{\mu \nu}(q, \omega) & = \sum_{\ell} Z_{\ell}^{\mu \nu}(q, \omega) \chi^{\ell}(q, \omega), \\
\chi^{\ell}(q, \omega) & = \sum_{\eta} \chi^{\ell}_{\eta}(q, \omega) \frac{g_{l}(k)}{v_{F \mu}(k)} Z_{\ell}^{\mu \nu}(q, \omega), \\
\chi^{\ell}_{\eta}(q, \omega) & = \frac{1}{V^2} \sum_{\mu} \int_{\mathbb{FS}} dS \Gamma_{k,k'} g_{l}(k') \frac{g_{l}(k)}{v_{F \mu}(k)} Z_{\ell}^{\mu \nu}(q, \omega).
\end{align}
essentially constant over the entire area, i.e., pair scattering processes involving all \( k_F \) momenta are relevant. The dominant pair fluctuations in the \( d_{\sigma} \) orbital channel (red) and in the \( d_{\pi} \) orbital channel (green) are highlighted. In the absence of orbital-selective QP-weight renormalization in the pairing kernel, i.e., starting from a model with \( Z_F = 1 \) for all orbitals \( \ell' \), Cooper pairing from the \( d_{\pi} \) orbital strongly dominates, leading to a pair fluctuation-like approach to pairing in infinite-layer nickelates [22,27–30,33]; for a comparison see the Supplemental Material [61]. But increasing effects of correlations in the pairing and thereby proportionally reducing the respective QP weight \( \sqrt{Z_{F\ell}} \) for orbital \( \ell' \) to \( \alpha(\sqrt{Z_{F\ell}}-1)+1 \) where \( \alpha \in [0...1] \), the \( d_{\pi} \) orbital maintains significant coherence at low energies because it is not close to a Mott-critical regime. This results in a leading \( s_\pm \) wave pairing instability displayed in Fig. 3(c) with sign changes between the red parts of the inner FS sheet and the pockets close to \( (\pi,\pi,\pi) \), driven by the \( (\pi,0,q_z) \) magnetic fluctuations. Importantly, this state remains nodal with vanishing gap on the large FS sheet; see Fig. 3(c). When reducing QP weights further, \( \alpha \to 1 \), i.e., \( Z_{F\ell} = Z_{F\ell}^0 \), surprisingly, the dominant instability is an odd-parity spin-triplet nodal SC state with \( p_z \) symmetry [see Fig. 3(d)], exhibiting again a full gap on the \( d_{\pi} \) dominated FS. At present, there are controversial reports on Pauli-limited superconductivity [9,12] such that a triplet state may be realized in infinite-layer nickelates. Finally, we note an interesting subleading even-parity two-dimensional \( g_{y3} : d_{x^2} / d_{x^2} \) state is close by in energy, but does not become leading for the parameter regimes we have explored in this Letter. Additional discussion on this state, the parameter dependence of our results, and the stability of the triplet state are presented in the Supplemental Material [61].

Superconducting spectral properties.—Our important message is that incorporation of the 3D FS and the significant doping difference of the \( d_{\pi} \) vs \( d_{\pi} \) orbital channels lead to a transition in the fundamental pairing symmetry. Infinite-layer nickelates are thus distinct from cuprates, where \( d_{\pi} \) superconductivity is the sovereign ruler. They are instead more comparable to, e.g., iron pnictides [52,54] or \( Sr_3RuO_4 \) [57,64]. This highlights the possibility of accidentally degenerate SC symmetries and the need for careful comparison to experiments in order to pinpoint the SC order parameter symmetry.

Focusing on the low-energy spectral properties, Fig. 4 shows the orbital-resolved density of states (DOS) \( \rho(\omega) \) for the three cases displayed in Figs. 3(b)–3(d). Analyzing \( \rho(\omega) \) is crucial because the tunneling conductance in scanning tunneling microscope (STM) experiments is strongly influenced by the nature of the surface atoms [65]. Nickelate STM data have revealed a fully gapped "U-shaped" spectra on some surfaces, while "V-shaped" spectra, reminiscent of a nodal superconductor, are found on others [7]. It has been shown theoretically that spectra

FIG. 3. Pairing structure with correlations. (a) The FS exhibits weak Fermi velocity \( v_F \) anisotropy implying that the pairing interaction \( \Gamma_{k,k'} \) in both the \( d_{\pi,\pi} \) (green) and \( d_{\pi} \) (red) orbitals is active. (b) Effect of correlations on the gap symmetry function \( g(k) \) of the leading instability. Upon reducing the QP weights \( Z_F \) by tuning \( \alpha \), a \( d_{\pi} \) pairing instability (b) transitions into a sign-changing \( s_\pm \) state (c), and eventually into a spin-triplet \( p_z \) state (d). For (c), (d) the dominant pairing interactions are in the \( d_{\pi} \) orbital states. Black arrows in (b)–(d): dominating pairing interactions (projected to band space). Used parameters are \( \tilde{U} = 0.8U_c \) and \( J/\tilde{U} = 1/5 \).
can interpolate between the partial DOS of one or the other internal degree of freedom by variation of the tip position within the unit cell [66]. Similar effects are expected from a tip-sample distance variation or if other surface atoms are present. At the moment, an ab initio calculation using surface Wannier functions is out of reach since the details of the surface are unknown. However, examining \( \rho_x(0)/\rho_x(0) \) for the \( s_{\pm} \) state, Fig. 4(b), one observes a V-shaped nodal behavior for the \( d_{\pm} \) orbital and U-shaped DOS in the SD orbital. The \( d_{\pm} \) orbital has a very small gap and may not be tunneled into because of its in-plane structure. This should lead to a suppressed value of the wave functions toward the vacuum [64,67]. By contrast, the SD orbital states are hybridized Wannier functions with significant weight distant to the NiO plane [37] and may be responsible for the STM-observed full-gap conductance [cf. Fig. 4(b)] [7]. The same argumentation for the \( d_{\pm} \) SC order parameter would lead to the hardly gapped spectrum in Fig. 4(a) if the in-plane orbital component cannot be picked up by the STM tip. Finally, the low temperature \( T \) behavior of the penetration depth \( \lambda(T) \) can be used to quantify the QP excitation spectrum at low energies [10,11]. In the present case, the calculated nodal SC order parameters in a clean material lead to a linear dependence of \( \lambda(T) \) at low \( T \), as we have verified numerically. This seems consistent with recent experiments on optimally doped La and Pr nickelates [11] when taking into account disorder effects [68]. For Nd-based nickelates, however, the situation appears more complex [10].

**Conclusions.**—Guided by recent experimental findings reporting significance of magnetism in infinite-layer nickelates, we have applied a microscopic model to obtain the pairing kernel from magnetic fluctuations relevant to these materials. In line with earlier studies, \( d_{\pm} \) Cooper pairing is found as a prominent candidate SC state. However, as a function of enhanced electronic correlations, we have uncovered a tendency for these systems to transition from \( d_{\pm} \) order to nodal \( s_{\pm} \) superconductivity. This appears consistent with recent experiments finding evidence of partial full-gap spectral properties of the SC state of infinite-layer nickelates.

We acknowledge useful discussions with F. Jakubczyk. We thank P. Buzduga for her contribution in the data analysis of the theoretical RIXS spectra. A. T. R. and B. M. A. acknowledge support from the Independent Research Fund Denmark, grant no. 8021-00047B. I. M. E. and F. L. are supported by the German Research Foundation within the bilateral NSFC-DFG Project ER 463/14-1.

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