

A self-consistency test of internally antisymmetric nonunitary triplet pairing in LaNiX₂-inspired models

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(Dated: June 16, 2026)

Internally antisymmetric nonunitary triplet (INT) pairing has been proposed as a way to reconcile time-reversal-symmetry breaking, multigap thermodynamics, and apparently nodeless superconductivity in the LaNiX₂ family. The proposal is attractive because an equal-spin triplet can have even spatial parity when the pair wave function is antisymmetric in an orbital index. Here we test the mechanism as a self-consistent mean-field problem. Starting from a two-orbital Hubbard-Kanamori interaction, we derive the local INT channel, impose the corresponding nonunitary Bogoliubov-de Gennes gap, and then allow competing anomalous and normal fields to relax in toy and material-derived Hamiltonians. The imposed state has the expected split $\Delta\Delta^\dagger$, spin-resolved density-of-states asymmetry, and condensate spin polarization. The self-consistency tests are more restrictive. A scalar INT attraction can sustain pairing but does not freely select a nonunitary imbalance; a robust nodeless spectrum additionally requires spin-orbital texture that keeps INT-paired partner states inside the Fermi subspace. When the same diagnostics are applied to current spin-orbit-coupled LaNiC₂ and LaNiGa₂ Wannier survey Hamiltonians, neither reduced nor first full-basis calculations select a robust nonunitary INT branch. The resulting conclusion is negative at survey level: INT remains a coherent constrained channel and diagnostic ansatz, but the present local Hubbard-Kanamori-like material calculations do not derive it as the self-consistent ground state.

I. INTRODUCTION

Muon spin relaxation experiments report time-reversal-symmetry breaking (TRSB) in both noncentrosymmetric LaNiC₂ and centrosymmetric LaNiGa₂ [1, 2]. At the same time, thermodynamic and penetration-depth measurements point to multigap and largely nodeless superconductivity [3, 4]. This combination is difficult to accommodate in a conventional single-band triplet picture, where nonunitary triplet states normally carry odd spatial parity and tend to have nodal structures constrained by crystal symmetry [5].

The internally antisymmetric nonunitary triplet proposal resolves the exchange-symmetry problem by using an additional orbital label [2, 3, 6]. The Cooper pair is spin triplet and equal-spin, but its orbital part is antisymmetric, allowing an even-parity local gap. If the two equal-spin amplitudes are unequal, the condensate is nonunitary and can carry a spin-polarized TRSB signature. The scenario is therefore a natural bridge between the experimental facts: two gaps, weak spontaneous fields, and no obligatory line nodes.

The question addressed here is narrower than the phenomenology. We ask whether the INT state follows as a self-consistent solution of a local two-orbital interaction and of material-derived LaNiX₂ normal-state Hamiltonians. This is a stricter test than imposing the gap. An imposed nonunitary order parameter may reproduce the desired signatures, but a microscopic derivation must also show that the freely relaxed anomalous and normal fields select the nonunitary branch over singlet, unitary triplet, and mixed competitors.

Our answer is cautious and negative. The local INT channel is well defined, and the imposed INT state

gives the expected nonunitary diagnostics. However, the present self-consistent toy calculations relax toward unitary or non-INT branches unless an explicit nonunitary bias or spin-polarization feedback is supplied. The current material-derived LaNiC₂ and LaNiGa₂ spin-orbit-coupled Wannier survey Hamiltonians likewise do not stabilize a robust nonunitary INT branch. The LaNiGa₂ SOC input has only partial Γ -Z direct-band validation and a large Wannier spread, so this is not a final exclusion theorem. It is instead a survey-level self-consistency benchmark: under the tested local Hubbard-Kanamori-like assumptions, INT is a coherent constrained mechanism but not yet a derived material ground state.

II. MODEL AND INT CHANNEL

We use a two-orbital spinor

$$\hat{\Psi}_{\mathbf{k}} = (\hat{c}_{\mathbf{k}a\uparrow} \ \hat{c}_{\mathbf{k}a\downarrow} \ \hat{c}_{\mathbf{k}b\uparrow} \ \hat{c}_{\mathbf{k}b\downarrow})^T. \quad (1)$$

The minimal normal-state toy Hamiltonian is

$$h_0(\mathbf{k}) = \xi_+(\mathbf{k})\tau_0\sigma_0 + \xi_-(\mathbf{k})\tau_z\sigma_0 + v(\mathbf{k})\tau_x\sigma_0 + \lambda\tau_y\sigma_z, \quad (2)$$

where τ_i and σ_i act in orbital and spin space. The local interaction is the two-orbital Hubbard-Kanamori form [7, 8],

$$\hat{H}_{\text{int}} = \hat{H}_U + \hat{H}_{U'} + \hat{H}_J + \hat{H}_P, \quad (3)$$

with intraorbital repulsion U , interorbital density repulsion U' , Hund exchange J_H , and local pair transfer J_P . In the channel convention used here, the interorbital equal-spin triplet scale is

$$V_{\text{INT}} = U' - J_H. \quad (4)$$

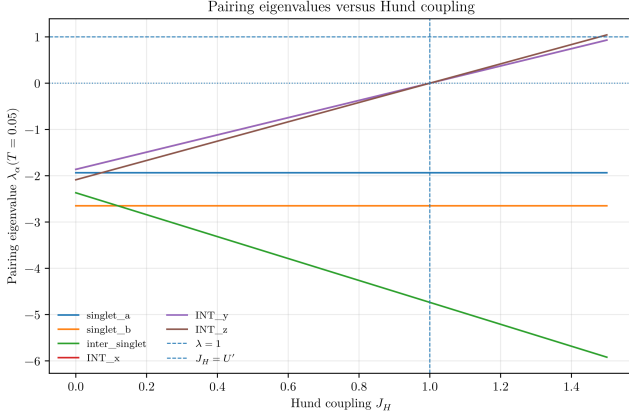


FIG. 1. Linearized local-channel diagnostic. Hund exchange favors the internally antisymmetric equal-spin triplet sector relative to interorbital singlet competitors, but the conservative bare hierarchy remains repulsive unless $J_H > U'$ or an effective attractive INT vertex is supplied.

Hund exchange therefore lowers the INT channel relative to interorbital singlets, but the bare local channel is attractive only in the strong hierarchy $J_H > U'$. For realistic repulsive parameters the INT sector can be the most favorable triplet descendant without being an instability by itself.

The imposed local INT gap is

$$\Delta_{\text{INT}} = \begin{pmatrix} 0 & 0 & \Delta_{\uparrow\uparrow} & 0 \\ 0 & 0 & 0 & \Delta_{\downarrow\downarrow} \\ -\Delta_{\uparrow\uparrow} & 0 & 0 & 0 \\ 0 & -\Delta_{\downarrow\downarrow} & 0 & 0 \end{pmatrix}. \quad (5)$$

The minus signs enforce antisymmetry under exchange of the two orbital labels. The state is nonunitary when

$$i\mathbf{d} \times \mathbf{d}^* \neq 0, \quad (6)$$

or equivalently when $\Delta_{\text{INT}}\Delta_{\text{INT}}^\dagger$ is not proportional to the identity in the paired subspace [5, 9]. In the Bogoliubov-de Gennes (BdG) problem,

$$\mathcal{H}_{\text{BdG}}(\mathbf{k}) = \begin{pmatrix} h_0(\mathbf{k}) + \phi(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta^\dagger(\mathbf{k}) & -h_0^T(-\mathbf{k}) - \phi^T(-\mathbf{k}) \end{pmatrix}, \quad (7)$$

both the normal field ϕ and anomalous field Δ must be updated from the density matrix and Gor'kov contraction in a self-consistent calculation.

III. FERMI-SURFACE PROJECTION

Channel selection is not enough. The gap that matters for weak pairing is the projection of the local matrix into the Fermi subspace,

$$\Delta_F(\mathbf{k}) = P_F(\mathbf{k})\Delta_{\text{INT}}P_F^T(-\mathbf{k}). \quad (8)$$

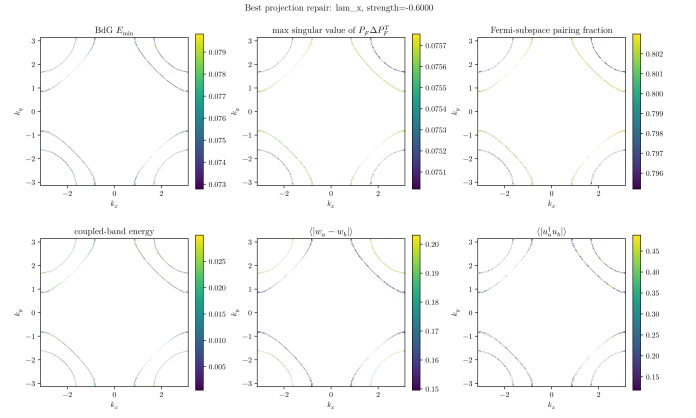


FIG. 2. Fermi-surface projection repair. The minimal toy model requires transverse spin-orbital texture to keep INT-paired partner states in the low-energy subspace. Increasing scalar attraction alone does not solve this projection problem.

In the minimal Hamiltonian of Eq. (2), the local INT matrix can be large while its same-Fermi-subspace projection is small. The INT operator then connects a low-energy state mostly to a partner outside the Fermi window, producing a near-nodal spectrum even when the linearized INT channel is favorable.

This obstruction can be exposed analytically by keeping only local spin-orbit terms

$$h_{\text{rep}}(\mathbf{k}) = \xi(\mathbf{k})\tau_0\sigma_0 + \tau_y(\lambda_x\sigma_x + \lambda_z\sigma_z). \quad (9)$$

The helicity projectors are

$$P_\nu = \frac{1}{2} \left[1 + \nu\tau_y \frac{\lambda_x\sigma_x + \lambda_z\sigma_z}{\sqrt{\lambda_x^2 + \lambda_z^2}} \right], \quad \nu = \pm. \quad (10)$$

For the fixed INT convention used here, the nonzero singular values of $P_\nu\Delta_{\text{INT}}P_\nu^T$ scale as

$$s_\nu = \left| \Delta_x \frac{\lambda_x}{\sqrt{\lambda_x^2 + \lambda_z^2}} \right|. \quad (11)$$

A purely longitudinal spin-orbit texture, $\lambda_x = 0$, therefore leaves the same-helicity INT projection zero in this limit. A transverse spin-orbital component immediately repairs the weak-pairing gap.

IV. IMPOSED NONUNITARY DIAGNOSTICS

The imposed INT state has the expected algebraic and spectral signatures. The eigenvalues of $\Delta_{\text{INT}}\Delta_{\text{INT}}^\dagger$ split when $|\Delta_{\uparrow\uparrow}| \neq |\Delta_{\downarrow\downarrow}|$, and the BdG density of states becomes spin resolved. These are necessary checks: they show that the implemented gap is genuinely nonunitary and that the code path detects the intended TRSB-like observables.

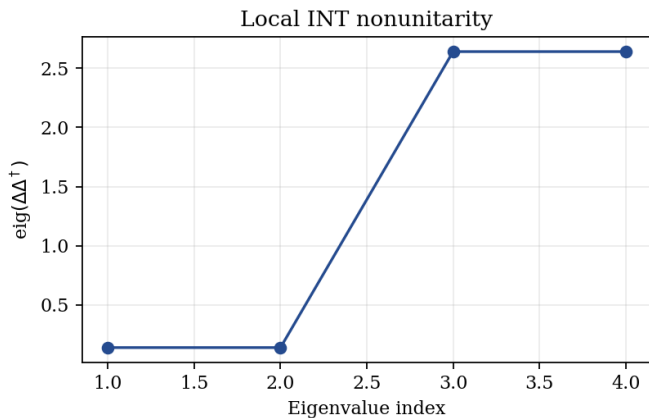


FIG. 3. Nonunitarity of the imposed INT gap. Unequal equal-spin components split the eigenvalues of $\Delta\Delta^\dagger$, the direct algebraic signature of a nonunitary triplet state.

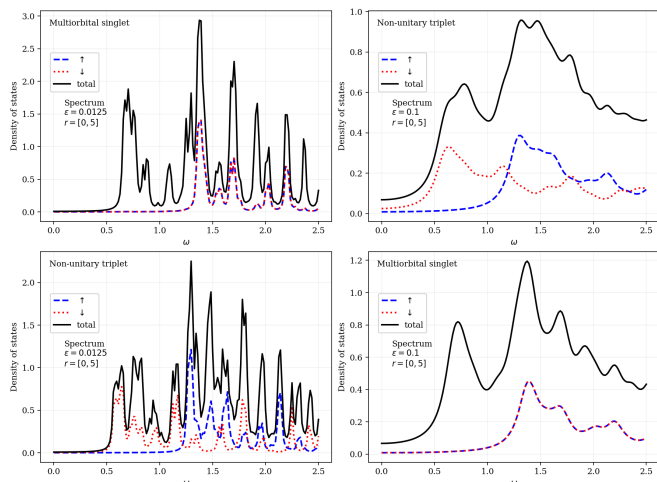


FIG. 4. Spin-resolved density of states for the imposed INT ansatz. The nonunitary gap produces a spin-resolved spectral asymmetry, but this imposed diagnostic does not by itself prove self-consistent phase selection.

The distinction between imposed diagnostics and phase selection is central. In a self-consistent calculation the fixed point

$$\mathcal{H}_{\text{BdG}}[\rho^{(n)}, \chi^{(n)}] \rightarrow \{\rho^{(n+1)}, \chi^{(n+1)}\} \rightarrow \{\phi^{(n+1)}, \Delta^{(n+1)}\} \quad (12)$$

must be allowed to choose among competing anomalous structures. The imposed nonunitary branch is a useful probe, but the relevant ground-state test is the free-energy ordering of relaxed singlet, unitary INT, nonunitary INT, mixed, and random seeds.

V. TOY SELF-CONSISTENCY

In the toy fixed-point tests, scalar INT attraction can sustain local interorbital triplet pairing. However, when

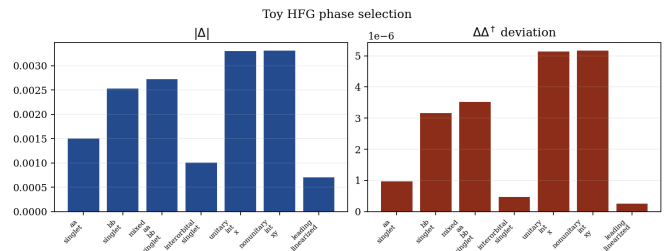


FIG. 5. Toy Hartree-Fock-Gor'kov phase selection. The constrained nonunitary branch is a diagnostic ansatz, while free relaxation favors a unitary or competing branch unless additional spin-polarization feedback is supplied.

the two equal-spin components are allowed to relax without an explicit nonunitary bias, the solution tends toward a unitary INT branch rather than a robust imbalance. Adding minimal Kanamori normal feedback does not change this qualitative outcome. The result is not a convergence failure: the iterations converge, but the nonunitary component is not freely selected.

This behavior is consistent with a Landau interpretation in which the total pairing amplitude and the nonunitary imbalance are distinct coordinates. The local triplet interaction can make the amplitude coordinate favorable while the imbalance coordinate remains penalized. A microscopic stabilization of nonunitarity therefore requires more than a scalar attractive INT vertex: it requires normal-state spin-orbital texture and interaction feedback that couple favorably to $id \times d^*$.

VI. MATERIAL-DERIVED LANIX₂ SURVEY

We next apply the same diagnostics to material-derived Wannier Hamiltonians. The current active inputs are spin-orbit-coupled Kent/Icarus survey Hamiltonians: LaNiC₂ with 88 spinor Wannier functions and 245 translation blocks, and LaNiGa₂ with 176 spinor Wannier functions and 125 translation blocks. The LaNiGa₂ SOC Hamiltonian was obtained from a random-start NSCF/Wannier continuation and has a large final spread of 523.69 square Angstrom. A direct QE-vs-Wannier smoke validation on the first Γ -Z high-symmetry segment gives a near- E_F RMSE of 0.135 eV, but fuller band-path validation attempts either ran too slowly or hit QE band-convergence failures. The material conclusions below should therefore be read as survey-level evidence.

The compact reduced-basis benchmark first keeps four near-Fermi states. In this reduced model the LaNiC₂ SOC survey has moderate INT projection and a unitary-INT-like best seed, while LaNiGa₂ SOC has stronger projection but selects an onsite-singlet-like branch after relaxation. In both cases the best nonunitarity is at numerical-noise scale.

Normal feedback was then included at three levels: anomalous-only BdG, density-density Kanamori

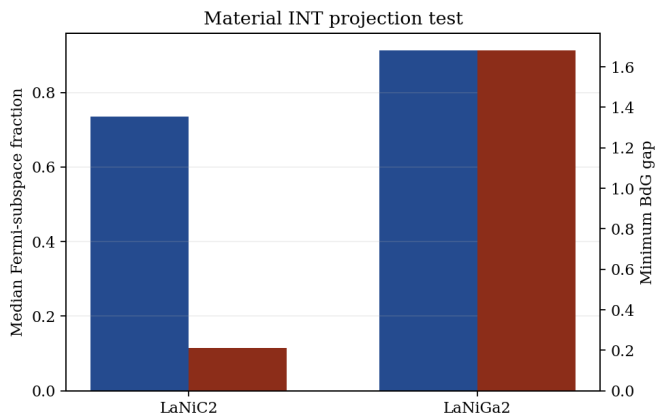


FIG. 6. Reduced material INT projection. The active LaNiGa₂ SOC reduction has substantial INT Fermi-subspace projection, but projection alone does not determine the relaxed phase.

TABLE I. Reduced material benchmark. The free-energy differences are relative to the normal reference in the compact scan.

| Material | translations | INT projection | best seed | nonunitarity |
|-------------------------|--------------|----------------|----------------|-----------------------|
| LaNiC ₂ SOC | 245 | 0.735 | unitary INT | 1.16×10^{-6} |
| LaNiGa ₂ SOC | 125 | 0.913 | onsite singlet | 7.64×10^{-7} |

Hartree feedback, and unrestricted compact Kanamori Hartree/Fock feedback. The normal feedback changes free energies and can move the best seed label, but it does not generate a clean nonunitary INT solution in the current material basis.

Finally, the same seed scan was repeated in the full active Wannier bases. This removes the most aggressive four-state truncation. Both active materials select onsite singlet rather than INT in the first full-basis scan, remain above the normal reference in the quick free-energy estimate, and have best nonunitarity at numerical-noise scale.

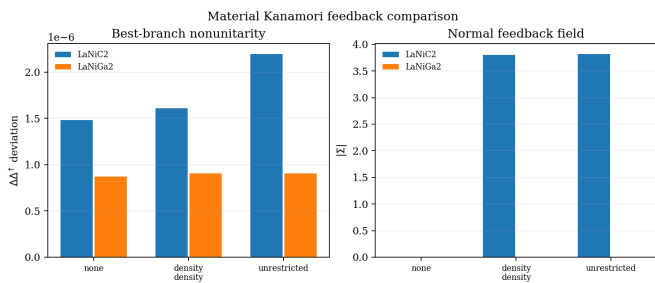


FIG. 7. Kanamori feedback comparison in the reduced material basis. Including normal-field feedback changes the compact free-energy landscape but does not stabilize a robust nonunitary INT branch.

TABLE II. First full-basis material seed scan. Both active spin-orbit-coupled survey Hamiltonians select onsite singlet in the current quick scan.

| Material | basis size | best seed | $\Omega - \Omega_N$ | nonunitarity |
|-------------------------|------------|----------------|-----------------------|-----------------------|
| LaNiC ₂ SOC | 88 | onsite singlet | 5.76×10^{-5} | 9.45×10^{-7} |
| LaNiGa ₂ SOC | 176 | onsite singlet | 3.40×10^{-5} | 6.82×10^{-7} |

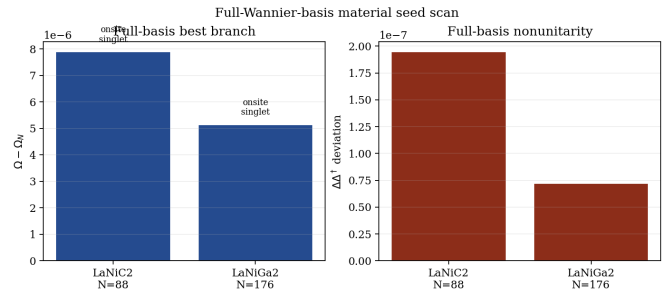


FIG. 8. Full-basis material seed scan. Keeping the full active Wannier basis removes the reduced four-state truncation and gives onsite-singlet-like winners for both LaNiC₂ and LaNiGa₂ SOC survey Hamiltonians.

VII. LIMITATIONS

The present result should not be overread. The material Hamiltonians are survey Wannier models with large spreads, not production-quality interpolations. The active LaNiGa₂ SOC basis has only a partial Γ -Z direct-band validation. The full high-symmetry validation path remains unresolved because the direct QE bands calculation is expensive and encountered `c_bands` nonconvergence on longer validation paths. The full interaction feedback is also incomplete at production scale: the compact tests include unrestricted Kanamori feedback, but the full-basis scans are still deliberately quick.

These limitations determine the correct interpretation. The calculations do not prove that INT is impossible in LaNiGa₂. They show that the specific route tested here—local Hubbard-Kanamori-like interactions applied to the current LaNiX₂ survey Hamiltonians—does not stabilize robust self-consistent nonunitary INT order. The next decisive calculation is a better-converged LaNiGa₂ SOC Wannier basis with full-path band validation and full-basis interaction feedback, not a broader search over unrelated toy models.

VIII. CONCLUSION

INT pairing remains a coherent and physically diagnostic channel. It is naturally connected to Hund-favored interorbital triplet pairing, and an imposed nonunitary INT gap gives the expected split $\Delta\Delta^\dagger$, spin-resolved density of states, and condensate spin polarization. The self-consistency tests are the restrictive step. Scalar

INT attraction does not by itself select a nonunitary imbalance, and current material-derived $\text{LaNiC}_2/\text{LaNiGa}_2$ survey Hamiltonians relax to unitary or onsite-singlet-like branches with nonunitarity at numerical-noise scale.

The defensible conclusion is therefore negative at survey level. The present calculations constitute a constrained derivation and falsification-style benchmark: they validate the INT ansatz as a channel and observ-

able diagnostic, but they do not derive it as a robust self-consistent material ground state under the tested local Hubbard-Kanamori-like assumptions.

ACKNOWLEDGMENTS

The numerical workflows and figures were generated from the QuLab research code base [10].

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