Pairing and isospin symmetry in proton-rich nuclei

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Abstract

Unlike their lighter counterparts, most odd-odd \( N = Z \) nuclei with mass \( A > 40 \) have ground states with isospin \( T=1 \), suggesting an increased role for the isovector pairing interaction. A simple SO(5) seniority-like model of this interaction reveals a striking and heretofore unnoticed interplay between like-particle and neutron-proton isovector pairing near \( N = Z \) that is reflected in the number of each kind of pair as a function of \( A \) and \( T \). Large scale shell-model calculations exhibit the same trends, despite the simultaneous presence of isoscalar pairs, deformation, and other correlations.

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With the advent of radioactive beams, unstable nuclei on the proton-rich side of the valley of stability are receiving increased attention. These nuclei will surely exhibit larger neutron-proton (np) pairing effects than do heavy stable nuclei, in which the valence protons and neutrons lie in different shells. This observation has been difficult to precisely quantify, however [1,2], despite many years of np-pairing theory [3]. The reason, as we shall see, is that in heavy nuclei with \( N \) near \( Z \), the delicate balance between like-particle (nn and pp) and np pairing has thus far partly eluded standard approximations.

In this work we focus our attention on isovector pairing in the ground states of fp-shell nuclei with \( N \) not too much bigger than \( Z \). Low-lying excited states are also interesting, but ground states deserve special attention because they determine masses and lifetimes. Our primary motivation for addressing isovector pairing is that unlike their lighter counterparts odd-odd fp-shell nuclei with \( N = Z \) usually have ground-state isospin \( T = 1 \). This suggests that the ground-state effects of isovector pairing are larger in the heavier nuclei, and perhaps not only when \( N \) is precisely \( Z \). Although isoscalar pairing obviously should not be neglected where np correlations are likely to be important, isovector pairing, which also generates np correlations, clearly deserves close examination in proton-rich nuclei.

Isospin symmetry dictates the relative strengths of the nn, pp, and np parts of the isovector pairing interaction. Unfortunately the generalized Hartree-Fock-Bogoliubov (HFB) methods typically used to treat pairing break isospin symmetry, and except in the \( N = Z \) nuclei the lowest-energy \( T = 1 \) pairs usually contain no np correlations\(^1\). Even in \( N = Z \) nuclei the method tends not to mix the np isovector pairs with the like-particle pairs, giving two degenerate states instead. Although we argue later that projecting HFB wave functions onto states with good isospin will allow such mixing, this procedure has never been systematically implemented [4] and the role played by \( T = 1 \) np pairing is therefore not fully appreciated. Here we examine the interplay between the different kinds of isovector pairs with techniques that conserve isospin from the start. We will see that like-particle and np pairing compete in a subtle but clearly visible fashion.

We proceed essentially in two steps. First we analyze the situation in an exactly solvable model that gives us some insight into precisely how the different kinds of pairs compete. We then show that the same patterns of competition are also present in realistic large-basis shell model calculations. The similarity between the results of a simple model and those of complicated numerical calculations that include many other effects besides isovector pairing strongly suggests that the patterns we describe here are quite general, and should also be present in real nuclei. After discussing how HFB theory might be altered slightly to capture these patterns, we conclude with a brief discussion of possible evidence for simple np isovector-pairing effects in binding energies.

We begin with the simple isovector-pairing model. We consider a single \( j \) orbital or a degenerate set with a total of \( 2\Omega \) \( m \)-substates and the pure isovector pairing interaction

\[
H = -G \vec{S}^\dagger \cdot \vec{S},
\]

\[
S^\dagger_M = \sum_{j,m>0} [a^\dagger_m a^\dagger_{m'}]_{M}^{T=1},
\]

\(^1\)The only exceptions of which we are aware are in Ref. [2], but there the authors break isospin symmetry completely by using \( T = 1 \) np pairing to represent \( T = 0 \) pairing.
where \( m \) is the \( z \)-projection of the angular momentum in a single-particle state, \( \bar{m} \) labels the corresponding time-reversed state, \( G \) is an arbitrary constant, and the square brackets indicate isospin coupling, so that \( S_M^1 \) is an isovector pair creation operator with projection \( M \). Together with the isospin and number operators, the angular-momentum-zero pair creation and annihilation operators above form the algebra \( SO(5) \). The Hamiltonian in Eq. (1), a generalization of the like-particle \( SU(2) \) seniority interaction, is solvable analytically. The space of fully-paired states in which the Hamiltonian acts is spanned by the set \( |\Omega, \mathcal{N}, T, T_z\rangle \), where \( \mathcal{N} = n/2 \) is half the total number of particles, \( T \) is the nuclear isospin, and \( T_z = 1/2(N - Z) \) is its \( z \)-projection. Algebraic techniques for computing matrix elements of operators between these states have existed for some time [5–7].

To quantify the effects of the different pairing modes, we define the operators
\[
N_{pp} = \frac{S_{-1}^1 S_1^1}{\Omega}, \quad N_{nn} = \frac{S_{-1}^1 S_{-1}^1}{\Omega}, \quad N_{np} = \frac{S_0^1 S_0^1}{\Omega},
\]
the sum of which enters \( H \) in Eq. (1). These operators are rough measures of the numbers of \( nn, pp \) and \( np \) pairs; their expectation values are related to the usual pairing gaps of the HFB theory. In the limit of large \( \Omega \), the pair-creation operators \( S_j^1 \) and their conjugates obey boson commutation relations, and the three operators just defined count the number of different kinds of bosons. To leading order in \( 1/\Omega \), the expectation values of these “number operators” therefore sum to \( \mathcal{N} \) and reproduce the results of Ref. [8], in which similar quantities (e.g. the total number of \( np \) bosons) are computed in the \( SU(3) \) limit of the \( IBM-4 \). With the generalized Wigner-Eckart theorem and the \( SO(5) \) Wigner coefficients tabulated in [7], we can obtain exact matrix elements for these operators, valid to all order in \( 1/\Omega \), between states with arbitrary values of \( \mathcal{N}, T, \) and \( T_z \). All even-even nuclei, which we examine first, have ground-state isospins \( T = T_z \); for these the “number operators” have the ground state expectation values (with \( N \geq Z \))
\[
\langle N_{np} \rangle = \frac{\langle N \rangle - T}{2T + 3} \left( 1 - \frac{N - T - 3}{2T} \right),
\]
\[
\langle N_{pp} \rangle = (T + 1) \langle N_{np} \rangle,
\]
\[
\langle N_{nn} \rangle = \langle N_{pp} \rangle + T(1 - \frac{N - 1}{\Omega}).
\]

These expressions are striking. Not surprisingly, when \( T = 0 \), i.e. \( N = Z \), all three expectation values are equal. But adding just a single pair of neutrons so that \( T = T_z = 1 \) causes the number of \( np \) pairs to drop by about 40%, while the number of \( pp \) pairs actually increases by about 7% (the number of \( nn \) pairs, naturally, increases even more). This result, which in the boson limit is due solely to the algebra of the 3-dimensional harmonic oscillator, fully captures the subtle competition between the three pair condensates. Increasing the number of neutron pairs increases the collectivity of the neutron condensate, making fewer neutrons available to pair with protons. As a result the protons pair more often with one another, even though their number hasn’t increased, and the binding in the \( np \) condensate drops dramatically. The right side of Fig. 1 shows what happens as \( T \) gets larger still: the trends continue to very large \( T \), where the state is nearly a product of \( nn \) and \( pp \) condensates. These results contrast with those of existing calculations [9–11], which as we have noted rarely
exhibit coexistence between like-particle and \( np \) isovector pairs (Ref. \[1\] applies HFB theory to the same model described here).

Interestingly, a generalization of \( SO(5) \) seniority to an \( SO(8) \)-based model that includes isoscalar pairing \([2]\) shows the pattern of isovector pairs to be relatively insensitive to the strength of the new mode, unless the latter is completely dominant \([10]\). In other words, the relative numbers of isovector \( np \), \( pp \), and \( nn \) pairs don’t change substantially (though the absolute numbers can) from the predictions above when an entirely different interaction is added, suggesting that the footprints of isovector pairing are not easy to erase. Realistic shell-model calculations in proton-rich \( fp \) shell nuclei bear this prediction out remarkably. Such calculations are difficult because of the size of the \( fp \) model space \([11]\), and only with the advent of the Shell Model Monte Carlo (SMMC) method have they begun to include the entire shell for nuclei heavier than \( A = 50 \) \([12]\). Performed with the modified Kuo-Brown interaction KB3, the SMMC calculations reproduce the general properties of these nuclei quite well \([13]\). The calculated total \( B(E2) \) and Gamow-Teller strengths agree particularly well with data, indicating that both isovector and isoscalar pairing are realistically described. Alongside the scaled predictions of the simple \( SO(5) \) model, we display in Fig. 1 results of the SMMC (with the same input and computing procedure as in Refs. \([13,14]\)) for the “number” of \( nn \), \( pp \), and \( np \) isovector pairs multiplied by \( \Omega \) in the Cr and Fe isotopes. Although the curves produced by the two models are not identical, they are strikingly similar; the additional physics in the shell model calculation — several orbits, isoscalar pairing, spin-orbit splitting, long-range correlations, deformation, etc. — reduce the total number of isovector pairs without dramatically changing their relative number. [The kinks in the SMMC \( N_{nn} \) curves reflect the closing in \(^{54}\text{Fe} \) and \(^{52}\text{Cr} \) of the \( f_{7/2} \) subshell.] The stubborn persistence of the patterns in all kinds of calculations strongly suggests that real nuclei exhibit them as well.

What about the \( N = Z \) nuclei in the \( fp \) shell, the ground state isospins of which are the clearest signal of \( np \) isovector pairing? How is the fact that the odd-odd nuclei have \( T = 1 \) reflected in the \( nn \), \( pp \), and \( np \) condensates? Intuition suggests that the extra isovector neutron-proton pair should give the \( np \) mode a slight advantage in its competition with like-particle pairing, and in the seniority model it clearly does. For states with \( T = T_z + 1 \), the model predicts

\[
\langle N_{np} \rangle = \frac{(3N + 3 - T) \left( 1 - \frac{N-T-3}{2\Omega} \right)}{2T + 3} - \frac{N + T + 1}{2\Omega},
\]

\[
\langle N_{pp} \rangle = \frac{(N - T) T \left( 1 - \frac{N-T-3}{2\Omega} \right)}{2T + 3},
\]

\[
\langle N_{nn} \rangle = \frac{[(N + T + 1) T - 3] \left( 1 - \frac{N-T-3}{2\Omega} \right) - (T - 1)(N + T + 1)}{2T + 3}.
\]

In the odd-odd \( N = Z \) nuclei with \( T = 1 \), these expressions imply more \( np \) pairing than in the even-even \( N = Z \) nuclei. Fig. 2 shows \( \langle N_{np} \rangle \) and \( \langle N_{nn} \rangle = \langle N_{pp} \rangle \) as a function of mass number when \( N = Z \); a characteristic odd-even staggering from the additional \( np \) pair in the odd-odd nuclei is the salient feature. As before, we find that this pattern also appears, though less prominently, in the SMMC calculations, the results of which are displayed in the same figure. Isoscalar pairing, which by itself produces smoother curves, may be partly
responsible for deviations from the simple formulae in Eq. (4), but it does not erase the staggering produced by isovector pairing.

As noted above, the reason isovector np correlations have gone largely unnoticed is that HFB theory as applied thus far does not mix them with nn and pp pairs. It also rarely lets isoscalar and isovector pairs coexist \[10,15\], instead (usually) assigning each \( N \approx Z \) nucleus three separate states: one with no np pairs, the second composed entirely of \( T = 1 \) np pairs and degenerate with the first, and the third containing only \( T = 0 \) pairs \[10,15\] and lying higher or (usually) lower in energy. Since the characteristic odd-even staggering results from mixing the first two solutions, it is not present in any of the three individually. We strongly suspect, however, that the restoration of isospin symmetry in HFB theory will at least partly correct these problems. To verify this conjecture we have reexamined the HFB treatment of SO(5), the existing version of which shows no neutron-proton correlations \[1\].

Restoring the symmetry means viewing the symmetry-violating quasiparticle vacuum as an intrinsic state in isospin space. From this vantage point \( T_z \) plays the role of the rotational quantum number \( K \) that labels bandheads. The usual constraint that \( < T_z >= N - Z \) (the analog of the rotational quantum number \( M \)) should therefore be eliminated or replaced. Here we assume “axial symmetry”, i.e. an intrinsic HFB wave function of the form

\[
|\text{HFB(intr)}\rangle = \exp \left[ \alpha S_0^+ \right] |0\rangle ,
\]

with \( \alpha^2 \) fixed at \( 2\mathcal{N}/(2\Omega - \mathcal{N}) \) by the usual constraint on the average total nucleon number. We project approximately by multiplying the intrinsic state by a “collective” rotational wave function \( D_{T_z,0}(\Omega)^* \) (where \( \Omega \) now stands for a rotation), in analogy with the Nilsson model. Continuing the analogy we assign the “number operators” intrinsic and collective parts as well, and for \( T = T_z \) obtain, e.g.,

\[
\text{projected HFB} : \langle \mathcal{N}_{np} \rangle \approx \frac{\mathcal{N} (1 - \mathcal{N}^2)}{2T + 3} + \mathcal{O}(\mathcal{N}^2/\Omega^2).
\]

This result makes perfect sense because the Nilsson prescription approximates projection only when \( \mathcal{N}, \Omega >> T \). The last term above, which also appears in the BCS approximation for like-particle pairing, is therefore much smaller than the others. Complete projection should add the missing factors of \( T \) so that the exact expression for \( \mathcal{N} \) in Eq. (3) is reproduced up to terms of order 1 or less. This kind of procedure may also facilitate the more complicated dynamical mixing of \( T = 1 \) and \( T = 0 \) pairs \[10\], in part because eliminating the traditional constraint on \( T_z \) allows a more general quasiparticle vacuum. Isospin projection in HFB theory clearly merits further study.

In concluding we return to the physical results obtained above: fp-shell nuclei exhibit striking and easily understood variations in the numbers of isovector nn, pp, and np pairs. We strongly suspect that the competition between the different kinds of pairs affects measurable properties of real nuclei. Unfortunately the heavy proton-rich nuclei are quite short-lived and few data are available to confirm this belief. Some structural information, however, can be gleaned solely from binding energies, which beside lifetimes are the most systematically measured quantities in these unstable nuclei and should be affected by pairing. A recent paper \[17\] points out that in sd-shell and p-shell nuclei the quantity \( \delta V_{np}(N, Z) \), defined as

\[
\delta V_{np}(N, Z) \equiv \frac{1}{4} \left\{ [B(N, Z) - B(N - 2, Z)] - [B(N, Z - 2) - B(N - 2, Z - 2)] \right\},
\]

is
where $B$ means binding energy and $N, Z$ are both even (similar quantities can be constructed for the other nuclei) is much larger when $N = Z$ than when $N \neq Z$. The paper then shows that this pattern follows from $SU(4)$ symmetry and argues that though apparently broken badly, primarily by spin-orbit splitting, the symmetry is therefore in some sense good. Here we note first that the combination in Eq. (7) is also enhanced for $N = Z$ in the heavier nuclei with $40 \leq A \leq 64$, so that the argument’s range of validity is even larger than claimed. We find in addition, however, that the preference for $N = Z$ is not an exclusive feature of $SU(4)$ symmetry; the same nuclei are in fact equally preferred in the pure isovector-seniority model discussed above. Though this fact doesn’t by itself prove that isovector neutron-proton pairing plays the visible role presented here, it is nonetheless suggestive and should motivate a greater effort to understand the properties of proton-rich nuclei, especially in regions that are still outside the ambit of shell-model calculations. The nuclei at the edge of stability will come under increasing experimental scrutiny, and the apparent validity of simple models (and dynamical symmetries) makes them all the more interesting.

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FIGURES

FIG. 1. The quantities $\Omega\langle N_{pp}\rangle$, $\Omega\langle N_{nn}\rangle$, and $\Omega\langle N_{np}\rangle$ for Fe and Cr isotopes, as a function of $N - Z = 2T_z$. On the left are the results of the Shell Model Monte Carlo calculation, and on the right are those from Eq. (3) (with $\Omega = 10$, half the number of single-particle levels in the $fp$ shell) scaled by a factor 0.5 to account for the reduction of the single-particle level density near the Fermi level and other effects.

FIG. 2. The quantities $\Omega\langle N_{pp}\rangle \equiv \Omega\langle N_{nn}\rangle$ (top panel), and $\Omega\langle N_{np}\rangle$ (bottom panel) for $N = Z$ nuclei. The full line connecting the points with error bars is the result of the Shell Model Monte Carlo calculation, and the dashed line is from Eqs. (3) and (4), again scaled by a factor 0.5.
