Systematic study of isoscalar and isovector pairing in the $2p1f$ shell

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Abstract. A systematic study of isoscalar and isovector pairing in $2p1f$ shell nuclei is reported, based on a model that includes deformation, isoscalar and isovector pairing and spin-orbit effects. Selected results are presented for three $N=Z$ nuclei, $^{44}$Ti, $^{46}$V and $^{48}$Cr, with a focus on the role of single-particle effects in dictating the competing pairing modes.

1. Introduction

In this paper, we review recent work [1] carried out to study the interplay of isoscalar and isovector pairing correlations in atomic nuclei with $N \approx Z$. Our analysis is carried out in the context of the nuclear shell model, which permits us to address the competition between these different modes of pairing in the presence of nuclear deformation and with all symmetries preserved.

The structure of the paper is as follows. In Section 2, we provide a brief historical overview of pairing in nuclei, including not only the usual $nn$ and $pp$ pairing that dominate in heavy systems but also $pn$ pairing as is in principle needed to describe nuclei near $N=Z$. In Section 3, we briefly describe the model that we use to investigate these competing pairing effects and then in Section 4 we report some selected results for several $N=Z$ nuclei in the $2p1f$ shell. Finally, in Section 5, we summarize the key conclusions that have emerged.

2. A brief historical overview

Pairing in nuclei derives from the short-range attraction between nucleons. Pairs of nucleons can get close together to optimize the strong short-range attractive force by rotating opposite one another, achieving net orbital angular momentum zero.

Pairing is traditionally described using Bardeen-Cooper-Schrieffer (BCS) theory [2], in terms of a condensate of collective Cooper pairs. Because of the small number of active nucleons that
can build pairing correlations, it is important to restore number conservation [3], which can be done using number-projected BCS theory [4].

Pairing correlations can also be combined with mean-field correlations, when necessary, through the use of Hartree Fock Bogolyubov (HFB) theory [5]. Now, however, angular momentum conservation is also lost and must be restored either exactly or approximately.

Since nucleons occur in two types ($n$ and $p$), they can form four distinct types of correlated (Cooper) pairs ($nn$, $pp$, or $pn$), each of which can in principle have net orbital angular momentum zero and thus exploit pairing correlations. In finite nuclei, however, the neutrons and protons must be in the same major shell if they are to exploit $pn$ pairing. Otherwise, only $nn$ and $pp$ pairing is important, as in typical nuclei with a neutron excess.

When $pn$ pairing is needed, i.e. when there is not a sizable neutron excess, BCS and HFB theory can be generalized to treat all pairing modes on an equal footing. Results based on the generalized HFB theory indicate that isoscalar $np$ pairing correlations are most important when $N \approx Z$ and when there are a reasonable number of valence neutrons and protons, precisely the regime in which quadrupole correlations are known to be important and where deformation is often present. Thus, it is important to include deformation in any analysis aimed at probing how the different kinds of pairing correlations compete in nuclear systems.

Nevertheless, there have been extensive studies of the different modes of pairing in model systems in which deformation is not present. In particular, the $SO(8)$ model [6], in which only $L = 0$ pairs contribute, has been used to obtain valuable information on the interplay of the different pairing modes. Despite the fact that the model does not contain deformation, except implicitly if the single-particle levels are not spherical, they nevertheless provide useful qualitative information. Such models, for example, make clear that generalized BCS (and thus HFB) theories cannot adequately treat the competing modes of pairing without restoration of symmetries, e.g. particle number, angular momentum and isospin [7].

For these reasons, we have chosen to study how the various modes of pairing compete in nuclear systems near $N = Z$ in the framework of the nuclear shell model, where it is possible to treat all pairing modes on an equal footing, preserve all symmetries and include the effects of deformation.

3. Our model

Our model consists of neutrons and protons restricted to the orbitals of the $2p1f$ shell outside a doubly-magic $^{40}$Ca core and interacting via a schematic hamiltonian

$$H = \chi \left( Q \cdot Q + a P^\dagger \cdot P + b S^\dagger \cdot S + \alpha \sum_i \vec{l}_i \cdot \vec{s}_i \right).$$

(1)

Here $Q$ is the mass quadrupole operator, $P^\dagger$ creates a correlated $L = 0, S = 1, T = 0$ pair, $S^\dagger$ creates a correlated $L = 0, S = 0, T = 1$ pair, and the last term is the one-body part of a spin-orbit force.

We carry out calculations as a function of the various strength parameters and for various nuclei. We start with pure $SU(3)$ rotational motion [8] associated with the $Q \cdot Q$ interaction and then ramp up the various $SU(3)$-breaking terms to assess how they affect the rotational properties.

4. Calculations

4.1. Optimal hamiltonian

It is interesting to first ask whether the hamiltonian (1) is capable of meaningfully describing the properties of nuclei in this region. With the parameters $\chi = -0.05$ $MeV$, $a = b = 12$, and $\alpha = 20$, we find an acceptable reproduction of all the spectra we have considered. This
Figure 1. Comparison of experimental spectra for $^{44}$Ti, $^{46}$Ti and $^{48}$Cr with the calculated spectra obtained using the optimal hamiltonian described in the text. All energies are in MeV.

is illustrated in figure 1 for $^{44}$Ti, $^{46}$Ti and $^{48}$Cr. The calculations reproduce the known non-rotational character of $^{44}$Ti and the highly rotational character known for $^{48}$Cr, including its observed backbend. We refer to $a = b$ as SU(4) pairing, from the dynamical symmetry that arises with this choice of parameters in the SO(8) pairing model [7].

4.2. $^{44}$Ti

We next focus on $^{44}$Ti, which has two active neutrons and two active protons outside the inert $^{40}$Ca core. In figure 2, we show the calculated energy splittings $E_I - E_{I-2}$ associated with the ground (YRAST) band as a function of the strength parameters $a$ and $b$ of isoscalar and isovector pairing, respectively. In these calculations we assume the optimal quadrupole strength of $\chi = -0.05$ MeV, but no spin-orbit interaction. What we see is that the isoscalar and isovector pairing interactions have precisely the same effect on the properties of the ground-state rotational band, in the absence of a spin-orbit interaction. This same conclusion was known from earlier works, and is confirmed here.

Next we show in figure 3 the corresponding results with the optimal spin-orbit term included. Now the symmetry between isoscalar and isovector pairing is broken, even though $^{44}$Ti has $N = Z$, and isovector pairing dominates.

4.3. $^{46}$V

Next we turn to $^{46}$V which has one additional neutron and one additional proton present. In figure 4, we show how the symmetry between isoscalar and isovector pairing in the absence of a spin-orbit force is reflected in this odd-odd $N = Z$ system. In the absence of isoscalar and isovector pairing, the $J = 1^+$ state and the $J = 0^+$ state form a degenerate ground state doublet. When only isoscalar pairing is turned on (panel a), the $J = 1^+$ state is pushed down below the $J = 0^+$ state. When only isovector pairing is turned on (panel b) the reverse happens and the $J = 0^+$ is pushed down and becomes the ground state. In the SU(4) limit (panel c) with equal isovector and isoscalar pairing strengths, the degeneracy reappears.

In figure 5, we show what happens in the presence of the physical spin-orbit interaction, for equal isovector and isoscalar pairing. Now the degeneracy is broken and the $0^+$ state emerges as the ground state, as in experiment. The experimental splitting is 1.23 MeV, whereas our optimal hamiltonian produces a slightly smaller splitting of 1.05 MeV.
Figure 2. Spectra of the ground band of $^{44}$Ti as a function of the strength of (a) the isoscalar pairing interaction and (b) the isovector pairing interaction, with no spin-orbit term present.

Figure 3. Spectra of the ground band of $^{44}$Ti as a function of the strength of (a) isoscalar pairing interaction and (b) the isovector pairing interaction, with the optimal spin-orbit term present.

4.4. $^{48}$Cr
Lastly, we consider $^{48}$Cr, which again has $N = Z$, but now with two quartet-like structures present. Here we assume as our starting point both the optimal quadrupole-quadrupole force and one-body spin-orbit force and then ramp up the two pairing strengths from zero to their optimal values. The results are illustrated in figure 6, for scenarios in which we separately include isoscalar pairing, isovector pairing and $SU(4)$ pairing with equal strengths. The experimental spectrum for $^{48}$Cr shows a backbend near $I = 12$, which is reproduced by our optimal hamiltonian. The results of figure 6 make clear that the backbend cannot be reproduced with pure isoscalar pairing, but requires isovector pairing as well.

The backbend in $^{48}$Cr was discussed earlier in the context of a shell-model study with a fully
Figure 4. Calculated energies of the lowest $J^\pi = 0^+$ and $1^+$ states of $^{46}$V with no spin-orbit term present, for (a) pure isoscalar pairing, (b) pure isovector pairing and (c) SU(4) pairing.

Figure 5. Calculated energies of the lowest $J^\pi = 0^+$ and $J^\pi = 1^+$ states of $^{46}$V as a function of the equal strengths of isoscalar and isovector pairing, with the optimal spin-orbit term present.
Figure 6. Calculated splittings in the $^{48}$Cr ground band, for isovector, isoscalar, and SU(4) pairing, respectively, as described in the text.

realistic hamiltonian in [9], where it was first shown to derive from isovector pairing. Our results are in agreement with that conclusion. To see these points more clearly, we show in figure 7 the numbers of isovector $S\dagger$ and isoscalar $P\dagger$ pairs as a function of angular momentum for the optimal hamiltonian. The pair numbers are obtained by evaluating $\langle S\dagger \cdot S \rangle$ and $\langle P\dagger \cdot P \rangle$ and scaling them with respect to the results that would derive from pure $T=1$ and $T=0$ pairing hamiltonians, respectively. As in ref. [9], the contribution of isovector pairing in the $J=0^+$ ground state is much larger than the contribution of isoscalar pairing. As the system cranks to higher angular momenta, the isovector pairing contribution falls off with angular momentum very rapidly eventually arriving at a magnitude roughly comparable with the isoscalar pairing contribution at roughly $J^{\pi}=10^+$. As the angular momentum increases even further we see a fairly substantial increase in the isovector pairing contribution at $J^{\pi}=12^+$, which according to figure 6 is where the backbend becomes prominent. After the backbend, both isoscalar and isovector pairing contributions decrease to near zero as alignment is achieved.

Since we have information not just on the states in the YRAST band but also on higher states as well, we can readily address whether the origin of the backbend that occurs in $^{48}$Cr in our calculations derives from band or level crossing. In figure 8, we compare the energies of states in the YRAST band with those of the lowest excited YRARE band, a $K=2^+$ band with similar intrinsic structure to the YRAST band. For the sake of comparison, we only show the
Figure 7. Calculated numbers of isovector $S^\dagger$ pairs and isoscalar $P^\dagger$ pairs in the ground (YRAST) band of $^{48}\text{Cr}$ for the optimal values of the hamiltonian parameters.

Figure 8. Calculated excitation energies of the ground (YRAST) band and the first excited (YRARE) band in $^{48}\text{Cr}$ for the optimal values of the hamiltonian parameters.
even angular momentum states in the YRARE band. As can be seen from the figure, the two bands get fairly close in energy near \( J = 6 \), which is well below the backbend. In the vicinity of the backbend, there is no evidence of the bands getting closer together in energy. On the basis of these results, we see no evidence that the backbend in the ground band of \(^{48}\text{Cr}\) derives from level crossing.

A possible hint as to where it might come from can be gleaned from a study of the pairing content of the two bands in the vicinity of the backbend. We already showed this information for the YRAST band in figure 7; in figure 9 we show the analogous information for the corresponding states in the YRARE band. In the YRARE band, as in the YRAST band, there is an increase in the number of isovector pairs in the vicinity of the backbend. In contrast, the number of isoscalar pairs does not change as dramatically in the YRARE band as in the YRAST band. Perhaps these results are suggesting that the backbend is driven by pairing, in some still to be defined way. We believe that these are interesting results, worthy of further study.

Figure 9. Calculated numbers of isovector \( S^1 \) pairs and isoscalar \( P^1 \) pairs in the first excited (YRARE) band of \(^{48}\text{Cr}\) for the optimal values of the hamiltonian parameters.

5. Summary
We have reported a shell-model study of proton-neutron pairing in 2\( p1f \) shell nuclei using a parametrized hamiltonian that includes deformation, spin-orbit effects and isoscalar and isovector pairing and is able to describe the evolution of nuclear structure in this region. Working in a shell-model framework, we were able to assess the role of the various modes of \( pn \) pairing in the presence of nuclear deformation without violating symmetries.

Some of the key conclusions that emerged are: (1) the symmetry between isoscalar and isovector pairing effects disappears already at \( N = Z \) in the presence of a spin-orbit force and isovector pairing dominates, (2) the fact that \(^{46}\text{V}\) has a \( 0^+ \) ground state derives from the spin-orbit interaction and its relative effect on isoscalar and isovector pairing, (3) isovector pairing dominates in \(^{48}\text{Cr}\) and produces its backbend, (4) the backbend in \(^{48}\text{Cr}\) does not derive from
the crossing of levels, and (5) isoscalar and isovector pairing exhibit a highly unusual behavior in the vicinity of the $^{48}$Cr backbend.

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