Proton-neutron pairing correlations in the nuclear shell model

S Pittel¹, Y Lei², N Sandulescu³, A Poves⁴, B Thakur¹ and Y M Zhao²

¹ Bartol Research Institute and Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716, USA
² INPAC, Department of Physics and Shanghai Key Lab for Particle Physics and Cosmology, Shanghai Jiao Tong University, Shanghai, 200240, China
³ Institute of Physics and Nuclear Engineering, 76900 Bucharest, Romania
⁴ Departamento de Fisica Teorica and IFT UAM/CSIC, Universidad Autonoma de Madrid, 28049, Madrid Spain.

E-mail: pittel@bartol.udel.edu

Abstract. Systematic shell-model calculations in 2p1f shell nuclei are reported, to assess the relative importance of isoscalar and isovector pairing in the presence of nuclear deformation and spin-orbit effects. Results are presented for three N = Z nuclei, ⁴⁴Ti, ⁴⁶V and ⁴⁸Cr.

1. Introduction
Pairing in nuclei is believed to derive from the short-range attraction between nucleons. To optimally exploit this force, nucleons form correlated Cooper pairs by rotating opposite to one another, thereby achieving net orbital angular momentum zero.

Since nucleons occur in two types (n and p), they can form several distinct types of Cooper pairs (nn, pp, or pn) with orbital angular momentum zero. In finite nuclei, however, the active neutrons and protons must be in the same major shell with N ≈ Z to exploit pn pairing. Elsewise, only nn and pp pairing will be important, as in those nuclei having a neutron excess.

Pairing correlations are traditionally treated using the Bardeen-Cooper-Schrieffer (BCS) approximation [1], in terms of a condensate of collective pairs. When necessary, mean-field correlations can be included on the same footing through the use of Hartree Fock Bogolyubov (HFB) theory [2]. In the presence of important pn pairing effects, BCS and HFB theory can be generalized to treat all pairing modes on an equal footing. Questions arise, however, as to whether these methods can adequately describe the physics of these competing modes without full restoration of symmetries [3].

The nuclear shell model, in contrast, can treat all pairing modes on the same footing without violation of symmetries. Furthermore, it can treat them in the presence of deformation, as is invariably important when N ≈ Z. We thus carried out a systematic study of the various modes of pairing in N ≈ Z nuclei in the 2p1f shell using the nuclear shell model [4]. In this paper, we briefly describe our model and report selected results of this study.
2. Our model

Our model consists of neutrons and protons restricted to the orbitals of the $2p1f$ shell outside a doubly-magic $^{40}\text{Ca}$ core and subject to 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 [5] associated with the $Q \cdot Q$ interaction and then systematically add the various $SU(3)$-breaking terms to assess how they impact the rotational properties.

3. Calculations

3.1. An Optimal hamiltonian

It is useful to note that the hamiltonian (1) is capable of meaningfully describing the properties of nuclei in this region. With the set of parameters $\chi = -0.05 \text{ MeV}$, $a = b = 12$, and $\alpha = 20$, we arrive at an optimal hamiltonian that acceptably reproduces the spectra of all nuclei we have studied, including the backbend that has been observed experimentally in $^{48}\text{Cr}$. We refer to the parameter choice $a = b$ as $SU(4)$ pairing, from the dynamical symmetry that arises with this choice of parameters in the $SO(8)$ pairing model [3].

3.2. $^{44}\text{Ti}$

The first nucleus we discuss is $^{44}\text{Ti}$, with two neutrons and two protons outside the $^{40}\text{Ca}$ core. Figure 1 shows the energy splittings $E_1 - E_{I-2}$ calculated for the ground (YRAST) band as a function of the parameters $a$ and $b$ of isoscalar and isovector pairing, respectively, with no spin-orbit interaction present. In these calculations we assume the optimal quadrupole strength of $\chi = -0.05 \text{ MeV}$. In such a scenario, i.e. in the absence of a spin-orbit interaction, the isoscalar and isovector pairing interactions have precisely the same effect on the properties of the ground-state rotational band. Though already known from earlier works, this conclusion also emerges clearly in our study.

In figure 2 we show the corresponding results with the optimal spin-orbit term included. Now the symmetry between isoscalar and isovector pairing is broken, even though $^{44}\text{Ti}$ has $N = Z$, and isovector pairing dominates.

3.3. $^{46}\text{V}$

Next we turn to $^{46}\text{V}$, with one additional neutron and one additional proton. In figure 3, 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 doublet. With only isoscalar pairing (panel a), the $J = 1^+$ state is pushed down below the $J = 0^+$ state. With only isovector pairing (panel b) the reverse happens and the $J = 0^+$ becomes the ground state. In the $SU(4)$ limit (panel c) with equal isovector and isoscalar pairing strengths, the degeneracy remains for all values of the common pairing strength.

Figure 4 shows what happens in the presence of the optimal spin-orbit interaction, for equal isovector and isoscalar pairing strengths. Now the degeneracy is broken and the $0^+$ state emerges as the ground state, as it does in experiment. The experimental splitting is $1.23 \text{ MeV}$, whereas our optimal hamiltonian produces a slightly smaller splitting of $1.05 \text{ MeV}$. 
Figure 1. Calculated energy splittings $E(I) - E(I - 2)$ (in MeV) in the ground band of $^{44}$Ti as a function of (a) the isoscalar pairing strength and (b) the isovector pairing strength, with no spin-orbit splitting. The pairing strengths are shown at the ends of the lines, as elsewhere in the manuscript.

Figure 2. 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.

3.4. $^{48}$Cr
Lastly, we consider $^{48}$Cr, which also 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 the optimal 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 5, for scenarios in which we separately include isoscalar pairing (panel a) and isovector pairing (panel b) and then in which we include $SU(4)$ pairing with equal strengths (panel c). As noted earlier, the experimental spectrum for $^{48}$Cr shows a backbend near $I = 12$. As is evident from panel c, this is nicely
Figure 3. 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 4. 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.
reproduced by our optimal hamiltonian. From figure 5 we conclude that the backbend in $^{48}\text{Cr}$ cannot be reproduced with pure isoscalar pairing, but requires isovector pairing as well.

The backbend in $^{48}\text{Cr}$ was discussed in a fully realistic shell-model study in ref [6], where it was first shown that it derives from isovector pairing. Our results support that conclusion. To see more clearly how these different pairing modes are reflected in the ground band, we show in figure 6 the number of isovector $S^\dagger$ pairs and the number of isoscalar $P^\dagger$ pairs as a function of angular momentum. As in ref. [6], 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, however, the isovector pairing contribution falls off 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 5 is precisely where the backbend occurs. After the backbend, both isoscalar and isovector pairing contributions decrease to near zero as rotational alignment is achieved.

Since our calculations provide information not just on the the YRAST band but also on higher bands, we can readily address whether the origin of the backbend that occurs in $^{48}\text{Cr}$ in our calculations derives from band or level crossing. In figure 7, we compare the energies of

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**Figure 5.** Calculated splittings in the $^{48}\text{Cr}$ ground band, for isovector, isoscalar, and SU(4) pairing, respectively, as described in the text.
Figure 6. Calculated numbers of isovector $S^\uparrow$ pairs and isoscalar $P^\uparrow$ pairs in the ground (YRAST) band of $^{48}$Cr for the optimal values of the hamiltonian parameters.

Figure 7. Calculated excitation energies of the ground (YRAST) band and the first excited (YRARE) band in $^{48}$Cr for the optimal values of the hamiltonian parameters.
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 even angular momentum states of the YRARE band. As can be seen from the figure, there is no evidence of the bands getting close together in energy in the vicinity of the backbend. On the basis of these results, we conclude that the backbend in the ground band of $^{48}$Cr does not seem to derive from level crossing.

Indeed, the only behavior that is unusual in the vicinity of the backbend is the substantial increase in the number of isovector pairs (and to a lesser extent isoscalar pairs) in that region. This seems to be further confirmation of the critical role of pairing correlations in producing the backbend in $^{48}$Cr and in our view merits further study.

4. Summary

We have reported a shell-model study of proton-neutron pairing in $2p1f$ shell nuclei using a Hamiltonian that includes deformation, spin-orbit effects and isoscalar and isovector pairing. By working in a shell-model framework, we can assess the role of the various modes of $pn$ pairing in the presence of deformation without violating symmetries.

Some of the key conclusions that emerged are: (a) the symmetry between isoscalar and isovector pairing effects disappears at $N = Z$ in the presence of a spin-orbit force and isovector pairing dominates, (b) that $^{46}$V has a $0^+$ ground state derives from the spin-orbit interaction and its relative effect on isoscalar and isovector pairing, (c) isovector pairing dominates in $^{48}$Cr and produces its backbend, (d) the backbend in $^{48}$Cr does not derive from the crossing of levels, and (e) isovector (and to a lesser extent isoscalar) pairing correlations exhibit a surprising behavior in the vicinity of the $^{48}$Cr backbend.

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