Systematic study of proton-neutron pairing correlations in the nuclear shell model

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Abstract. A systematic study of proton-neutron pairing in 1$f$ – 2$p$ shell nuclei is reported, based on a model that includes deformation, spin-orbit effects and isoscalar and isovector pairing. Selected results are presented for $^{44}$Ti, $^{46}$V and $^{48}$Cr.

1. Introduction
Proton-neutron (pn) pairing is generally thought to be important in nuclei with roughly equal numbers of neutrons and protons [1]. The standard technique for treating these correlations is through BCS or HFB approximation, generalized to include the pn pairing field in addition to the nn and pp pairing fields. It is not clear, however, whether these methods can adequately represent the physics of the competing modes of pair correlations without full restoration of symmetries [2]. To address this issue, we have carried out a systematic study of pairing correlations in nuclei in the context of the shell model, whereby all pairing modes can be treated on an equal footing and all symmetries preserved.

In Section 2 we briefly describe our model and in Section 3, we report some selected results we have obtained. Finally, in Section 4, we summarize the key conclusions that have emerged.

2. Our model
Our model consists of neutrons and protons restricted to the orbitals of the 1$f$ – 2$p$ 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 an $L = 0, S = 0, T = 1$ pair and the last term is the one-body part of a spin-orbit force.
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.

We carry out calculations as a function of the various strength parameters and for various nuclei. We start with pure SU(3) rotational motion 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.

3. Calculations

3.1. Optimal hamiltonian

We first ask whether the hamiltonian (1) is capable of describing nuclei in this region. With the parameters $\chi = -0.05$ MeV, $a = b = 12$, and $\alpha = 20$, we obtain an acceptable reproduction of all the spectra we have considered. This is illustrated in figure 1 for $^{44}$Ti, $^{46}$Ti and $^{48}$Cr. The calculations reproduce the non-rotational character of $^{44}$Ti and the highly rotational character of $^{48}$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 [2].

3.2. $^{44}$Ti

We next focus on $^{44}$Ti, with two active neutrons and two active protons. In figure 2, we show the calculated energy splittings $E_I - E_{I-2}$ associated with the ground-state band as a function of the strength parameters $a$ and $b$ of isoscalar and isovector pairing, respectively. In these calculations we assumed a quadrupole strength of $\chi = -0.05$ MeV and 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.

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

3.3. $^{46}$V

Next we turn to $^{46}$V with 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.
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.

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.

3.4. $^{48}$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
**Figure 4.** Calculated energies of the lowest $J^\pi = 0^+$ and $1^+$ states of $^{46}\text{V}$ 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 $1^+$ states of $^{46}\text{V}$ as a function of the equal strengths of isoscalar and isovector pairing, with the optimal spin-orbit term present.
isoscalar pairing, isovector pairing and SU(4) pairing with equal strengths. The experimental spectrum for $^{48}\text{Cr}$ 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.

**Figure 6.** Calculated splittings in $^{48}\text{Cr}$ ground band, for isovector, isoscalar, and SU(4) pairing, respectively, as described in the text.

The backbend in $^{48}\text{Cr}$ was discussed earlier in the context of a shell-model study with a fully realistic hamiltonian in [3], 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. [3], the contribution of isovector pairing in the $J = 0^+$ ground state in 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.
Figure 7. Calculated numbers of isovector $S^\uparrow$ pairs and isoscalar $P^\uparrow$ pairs in the ground (YRAST) band of $^{48}\text{Cr}$ for the optimal values of the Hamiltonian parameters.

4. Summary
We have reported a shell-model study of proton-neutron pairing in $1f - 1p$ 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, and (3) isovector pairing dominates in $^{48}\text{Cr}$ and produces its backbend.

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