Spin-aligned neutron-proton pair coupling in the era of large scale computing

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Abstract. Shell model calculations reveal that the ground and low-lying yrast states of the \( N = Z \) nuclei \(^{92} \text{Pd} \) and \(^{96} \text{Cd} \) are mainly built upon isoscalar spin-aligned neutron-proton pairs each carrying the maximum angular momentum \( J = 9 \) allowed by the shell \( 0g_{9/2} \) which is dominant in this nuclear region. This mode of excitation is unique in nuclei and indicates that the spin-aligned pair has to be considered as an essential building block in nuclear structure calculations. In this contribution we will discuss this neutron-proton pair coupling scheme in detail. It may help in understanding the intrinsic structure of the shell-model wave function. In particular, we will explore the competition between the normal monopole pair coupling and the spin-aligned coupling schemes.

The present version of nuclear shell model [1] was introduced at the same time as the invention of modern computer, the “Baby”, which was designed and built at The University of Manchester [2]. The nuclear shell model calculations involved large scale computing, even at the beginning of its development. The original work of Nilsson [3] was carried out on the BESK computer which was the largest one in Sweden available for scientific computation at that time [4]. Shell model Hamiltonian matrices up to dimension \( 10^{10} \) can now be handled. The purpose of these large scale computations is to gain insight on our understanding of the complicated shell model wave function. The essential ingredients of the shell model turned out to be the strong spin-orbit interaction and the seniority coupling in the \( jj \)-scheme. The seniority coupling dominates the low-lying states of semi-magic nuclei, where the driving force behind is the strong pairing interaction between like particles. Meanwhile, many open-shell nuclei have quadrupole moments that are much larger than could be attributed to a single particle, which implies the sharing of angular momentum between many particles. A remarkable feature of nuclear structure physics is that essential ingredients of the single-particle model could be retained by assuming that the nucleons move in an deformed average potential, which removes the spurious degrees of freedom corresponding to the collective spectrum [3].

Neutrons and protons can form neutron-proton (\( np \)) pairs with angular momenta \( J = 0 \) to \( 2j \) and isospin quantum numbers \( T = 0 \) (isoscalar) and \( T = 1 \) (isovector). The isovector \( np \) channel manifests itself in a fashion similar to like-nucleon correlations. There has been longstanding and intensive interest in exploring the signature of isoscalar \( np \) pairing (in particular \( np \) pairs with \( J = 1 \) and \( S = 0 \)) in the structure of self-conjugate nuclei [5, 6, 7, 8]. In this contribution we would like to discuss the so-called spin-aligned \( np \) pair coupling from a nuclear shell-model perspective. The spin-aligned pair may be considered as an essential building block in nuclear structure calculations. We will show that the aligned \( np \) pairs can generate striking regular
evolution patterns in the energy spectra and transition probabilities along the yrast states of $N=Z$ nuclei. These may be deemed as a new kind of collective mode with isoscalar character that is unique in the atomic nucleus. In a recent work the low-lying yrast states in $^{92}_{46}$Pd were observed and it was inferred that for the first time a transition from the isovector pair coupling mode to such spin-aligned $np$ coupling scheme may have occurred [9, 10].

As one would expect, near the closed shell nucleus $^{100}$Sn, i.e., in $^{96}$Pd ($^{98}$Cd) with four (two) proton holes outside of $^{100}$Sn, the positions of the energy levels correspond to a $(g_9/2)_{\lambda}^J$ pairing spectrum, as shown in Ref. [10]. When the number of neutron holes increases, the levels tend to be equally separated, which is a characteristic of vibrational spectra. This are specially the cases for $^{92}$Pd and $^{96}$Cd which show equally-spaced level schemes up to $I = 12$ and $I = 6$, respectively. Already the systematics of experimental data suggests gradual decrements in both the quadrupole deformation $\beta_2$ and $E(4_1^+)/E(2_1^+)$ ratio in $N = Z$ nuclei when approaching the $^{108}$Sn shell closure [11, 12]. To understand the yrast structures of $^{92}$Pd, $^{96}$Cd and neighboring nuclei, we perform nuclear shell model calculations within the $1f_{5/2}1p_{1/2}$ model spaces using the Hamiltonian given in Ref. [13] and a variety of other interactions which are quoted therein. In particular, we perform calculations using as single-particle states the orbits $pg$ and $0g_9/2$, with the interactions of Refs. [14, 15, 16], in order to explore the importance of configuration mixing in determining the structure of the spectrum.

In Table 1 we compare the strengths of the interaction matrix elements corresponding to different shell model spaces [13, 14, 16]. In the case of $0g_9/2$ space, only the relative strengths are given for simplicity. The absolute strength of the monopole centroid has no influence on the coupling of the wave functions and excitation energies. Also it should be mentioned that the relative strength of the $T = 0$ and $T = 1$ monopole interactions does not play any role on the structure of nuclear states. That is, the wave functions remain unchanged by adding a constant to the $T = 0$ or 1 part of the interaction. This modification only affects the relative energies of the states with different isospin quantum numbers. The matrix element for the $f_{pg}$ model space, for which we took from Ref. [13], are defined in the particle-particle channel by assuming $^{56}$Ni as the core. The mass dependence of the interaction is assumed to be $(A/58)^{-0.3} = 0.87$ for $A = 92$ where $A$ is the mass number of the nucleus to be calculated.

As mentioned above, present shell model calculations are able to include a large number of shells [17]. But our calculations tend to suggest that many properties of nuclei in this region can be explained by calculations restricted the the single $0g_9/2$ shell only. This does not mean that the other shells (the $0f_{1p}$ orbitals and even other higher lying shells) has no contribution to the wave function. But normally one may safely expect the effect from these shells can be taken into account through the renormalization of the effective interaction and effective operators (c.f., Table 1). The contributions from other shells may be deemed as the background whose effect on the nuclear structure is relatively harder to identify. This is because our knowledge of complex objects like atomic nuclei are obtained through systematic studies of neighboring states.

| Table 1. The $0g_9/2$ interaction matrix elements for different model spaces [13, 14, 16]. |
| Space | $J = 0$ | $J = 2$ | $J = 4$ | $J = 6$ | $J = 8$ | $J = 1$ | $J = 3$ | $J = 5$ | $J = 7$ | $J = 9$ |
|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| $0g_9/2$ | 0 | 1.458 | 2.283 | 2.549 | 2.688 | 1.220 | 1.592 | 1.882 | 1.930 | 0.626 |
| $pg$ | -2.089 | -0.919 | -0.094 | 0.172 | 0.311 | -1.038 | -0.785 | -0.495 | -0.447 | -1.751 |
| $f_{pg}$ | -1.691 | -0.959 | -0.087 | 0.152 | 0.269 | -1.138 | -0.599 | -0.383 | -0.561 | -2.207 |
As a result, only relevant degrees of freedom that distinguish one state from the others can be identified. Also full fp shell model calculation has been feasible for the nucleus \(^{48}\)Cr since almost 20 years ago. But it is realized that the \(0f_{7/2}\) and \(1p_{3/2}\) shells would be enough to explain the bulk properties of this deformed nucleus \([18]\). It is noted that, when the calculations are restricted to the \(0f_{7/2}\) shell only, both the \(N = Z\) nuclei \(^{44}\)Ti and \(^{48}\)Cr exhibit an equally-spaced pattern similar to the one obtained with the shell \(0g_{9/2}\). However, the aligned \(T = 0\) np coupling is not manifested in the spectra of the \(fp\) shell since the proximity of the shell \(1p_{3/2}\) and the strong quadrupole interaction thus developed leads to the mixing of shell model configurations that forms a more favorable description of deformed mean field. On the contrary, our calculations show that in the mass 90-100 region and the \(0g_{9/2}\) shell the quadrupole interaction with the \(1d_{5/2}\) level is not strong enough to scatter nucleons appreciably across the energy gap associated with the magic numbers \(N, Z = 50\). Work underway is to explore in a more quantitative way the influence of deformation on the aligned np pair coupling.

![Figure 1](image-url)

**Figure 1.** (Color online) Coefficients \(x^2\) corresponding to the \(|((\nu\pi)_9)^2; 0\rangle\) component in the wave functions of the first three \(T = 0\) states of \(^{96}\)Cd for each spin.

It is suggested that the apparent collectivity in the spectra of \(^{96}\)Cd and \(^{92}\)Pd may have a different origin than that resulting from a vibration or rotational motion usually attached to nuclear collective phenomena \([9, 10]\). Since there is no evidence for shell interferences in the spectra of Pd isotopes, we will analyze other sources which control the structure of those spectra, namely the different coupled pair modes. To probe the pair content in the many-fermion wave function \(\Psi\) one may evaluate the two-particle transfer amplitude \(\langle \Psi_N|\{a_i^\dagger a_j^\dagger\}, J\pi\rangle|\Psi_{N-2}\rangle\) or the average number of pairs \(\langle \Psi_N|\{a_i^\dagger a_j^\dagger\}, J\pi\times (a_i a_j), J\pi\rangle_0|\Psi_N\rangle\) or project the shell-model wave functions onto a pair coupled basis with the help of the two-particle coefficients of fractional parentage. In Refs. \([9, 10, 19]\) we applied the two-particle coefficients of fractional parentage technique. Two sets of the orthonormal bases are constructed starting from the monopole \(J = 0\) and \(J = 9\) pairs. In Refs. \([16, 20, 21]\) all possible combinations are considered within an non-orthogonal basis by applying the so-called multistep shell model. After projecting the yrast wave functions into a product of isoscalar \(J^\pi = 9^+\) pairs we found the most striking feature of this case: As can be seen from Fig. 1, all low-lying yrast states of \(^{96}\)Cd (and \(^{92}\)Pd) are built mainly from \(J^\pi = 9^+\) spin-aligned np pairs as \(|((\nu\pi)_J=9)^{N/2}\rangle\).
For systems with four pairs the total number of interacting pairs is \( N = n(n - 1)/2 = 28 \).

For a low-lying yrast state in \(^{92}\text{Pd}\) which has total isospin \( T = 0 \), the total number of isoscalar pairs is \( |n/2(n/2 + 1) - T(T + 1)|/2 = 10 \). If isospin symmetry is assumed, the numbers of isovector neutron-neutron, proton-proton and \( np \) pairs are the same and the total number of pairs is \( |3n/2(n/2 - 1) + T(T + 1)|/2 = 18 \). The results for the isoscalar pairs thus obtained in the \( pq \) space are shown in the left panel of Fig. 2. One sees that all low-lying yrast states are built mainly from \( J^\pi = 9^+ \) spin-aligned \( np \) pairs. We also calculated the numbers of isovector pairs in \(^{92}\text{Pd}\) in the right panel of Fig. 2. It is seen that already in the ground state we have much more pairs with \( J > 0 \) than the normal \( J = 0 \) pair. In particular, the dominating component is the \( J = 8 \) pair which is maximally aligned in the isovector channel. This is due to the large overlap between states generated by the spin-aligned \( np \) pairs and those generated by the isovector pairs. This phenomenon is not seen in systems with two \( np \) pairs where the contributions from the isovector aligned pair is practically zero for low-lying yrast states [16]. It should be emphasized that the dominating component in the wave functions of low-lying yrast states in \(^{92}\text{Pd}\) is still the spin-aligned \( np \) pair coupling. But it may be interesting to clarify the role played by the isovector aligned pair in \( N = Z \) systems with more than two pairs. Work on this direction is underway.

Calculations for the number of interacting pairs in the wave functions of \(^{96}\text{Cd}\) are plotted in Fig. 3. In this system with two proton holes and two neutron holes, we have three isoscalar and three isovector interacting pairs. In the \( T = 0 \) channel, all low-lying yrast states are built mainly from \( J^\pi = 9^+ \) spin-aligned \( np \) pairs. On the other hand, these states show a mixture of many components, in particular the \( J = 0 \) and \( 2 \) pairs. As noticed in Ref. [10], the \( 81^+ \) state in \(^{96}\text{Cd}\) corresponds to a normal seniority \( v = 2 \) coupling.

The four \( J = 9 \) \( np \) pairs in \(^{92}\text{Pd}\) can couple in various ways. With the help of two-particle cfp one may express the wave function in terms of \( (((\nu\pi)_9 \otimes (\nu\pi)_9)_{9'} \otimes (\nu\pi)_9)_{9''} \otimes (\nu\pi)_9)_J \). It is thus found that, among the various aligned \( np \) pair configurations, the stretch configuration, \( (((\nu\pi)_9 \otimes (\nu\pi)_9)_{16} \otimes (\nu\pi)_9)_{16''} \otimes (\nu\pi)_9)_J \), is calculated to occupy around 66\% of the ground state wave function of \(^{92}\text{Pd}\), i.e., with amplitude \( X(01^+_7) = 0.81 \) [10]. The maximal \( J = 24 \) state corresponds to a pure stretch configuration. On the other hand, by rewriting the wave function of \(^{92}\text{Pd}\) as a product of two group with two \( np \) pairs (i.e., \(^{96}\text{Cd} \) each) within an non-orthornormal basis it is thus found the leading component is the coupling \( |^{96}\text{Cd}(gs) \otimes ^{96}\text{Cd}(gs)\) as can also
Figure 3. Average number of isoscalar (upper) and isovector (lower) \( (0_{9/2}^2)_{J} \) interacting pairs as a function of total angular momentum \( I \) in the wave functions of the yrast states of \(^{96}\text{Cd}\).

Figure 4. Wave function amplitudes for the components \(|^{96}\text{Cd(gs)}\otimes^{96}\text{Cd(gs)}\rangle\) and \(|^{96}\text{Cd}(16^+)\otimes^{96}\text{Cd}(16^+)\rangle\) in the ground state wave function of \(^{92}\text{Pd}\) as a function of the ratio between the strengths of \(V_0\) and \(V_0\). The calculation is done in the \(0_{9/2}^2\) shell with all other matrix elements are set to zero.
be seen from Fig. 4.

It has to be mentioned that the simple arguments present in this contribution are mainly based on toy model calculations within one orbital. It may be useful in elucidating the structure properties of $N=Z$ and neighboring nuclei and the residual degrees of freedom. But one has to be aware that the real situation can be much more complex. Ongoing work is to generalize the aligned $np$ pair coupling to systems with many shells. This generalization may not be straightforward within the present shell model framework due to the fact that the corresponding aligned $np$ pairs can carry different angular momenta. One possibility to overcome this drawback is through introducing as building blocks four-body quartets which are composed of aligned $np$ pairs [22] (see, also, Fig. 4).

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