Complementarity and Competitiveness of the Pairing and Quadrupole Interactions in the Microscopic Shell Model

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Abstract. We explore the algebraic realization of the Pairing-plus-Quadrupole Model /PQM/ in the framework of the Elliott's SU(3) Model with the aim to obtain the complementary and competing features of the two interactions through the relation between the pairing and the SU(3) bases. First, we establish a correspondence between the SO(8) pairing basis and the Elliott's SU(3) basis. It is derived from their complementarity to the same LS-coupling chain of the shell-model number-conserving algebra. The probability distribution of the SU(3) basis states within the SO(8) pairing states is also obtained and allows the investigation of the interplay between the pairing and quadrupole interactions in the Hamiltonian of the PQM. Some particular examples based on this SO(8)-SU(3) basis correspondence are applied for the build-up of a more elaborated microscopic model that can be used in more realistic cases, which take into account the interactions between two shells and between a shell plus an orbital.

1 Introduction

The most important short- and long-range residual interactions in the nuclear structure physics are considered to be the pairing [1] and the quadrupole-quadrupole interactions [2] that have to be taken into account in the shell-model description of the nuclear systems [3]. This is the main assumption in the formulation of the Pairing-plus-Quadrupole Model /PQM/ [4-6] for the description of the nuclear excitation spectra. The basis employed in this case is the one of the deformed shell model, but the applications to real nuclear systems are rather complicated and cumbersome, due to the enormous dimensionality of the model space in particular for the heavy nuclei. Being with different range of action on the nucleons in the valence shells it is quite clear that these interactions actually influence the behavior of the systems in different parts of the shells. In such a case the problem is simplified by employing a group-theoretical approach [7], which introduces symmetry principles, useful in particular when identifying dynamical symmetries [8], which represent exactly solvable limiting cases of the model Hamiltonian. The PQM is particularly convenient for this purpose, since its basic interactions - the pairing and quadrupole are invariants of two respective algebras, which reduce the general symmetry of the

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shell model in a dynamical way. At the same time, it has been shown in [9] that the two so defined dynamical symmetry chains, are both complementary to the Wigner's spin-isospin $SU_{ST}(4)$ symmetry, which establishes the direct connection between these two limiting cases. The latter allows for the investigation of the competing and complementarity features of the pairing and quadrupole interactions in the description of the realistic nuclear systems in the lower shells up to mass numbers $A \sim 100$.

Another advantage of this approach is that it is rather general and works in any of the nuclear shells and also in only part of the shells, like a single orbital, which allows us to investigate how the model works not only in a single shell, but in two shells or in a shell plus a single orbital. Such an extension of the PQM will allow the consideration of a richer model space and the role of the intruder levels in the heavier shells. The aim of this work is to start with the investigation of these new features of the extended algebraic version of PQM and to prove its advantages in some simple applications to real nuclear systems.

2 Algebraic Structure of the Many-Particle Shell Model

$$\begin{cases} 1^{m} \} & U(4\Omega) \\ & \downarrow \\ \{\tilde{f}\} & [U(\Omega) & \otimes & U_{ST}(4)] & \{f\} \\ & \downarrow & \searrow \alpha & \downarrow \\ [\tilde{\mu}] & [SO(\Omega) & [SU(3) & \otimes & SU_{ST}(4)] & \{f'\} \\ (\nu[p]) & \Leftrightarrow SO(8) & (\lambda, \mu) & \sim SO(6) & [P] \\ \beta & \downarrow & \swarrow K & \downarrow \\ L & [SO_{L}(3) & \otimes & SU_{S}(2)] \otimes SU_{T}(2) & S, T \\ & \downarrow & \downarrow \\ J & SU_{J}(2) & \otimes SU_{T}(2) & T \end{cases}$$
(1)

We start with a short explanation and analysis of the reduction scheme (1) which gives the reduction of the algebraic realization of the shell-model algebra

$$U(4\Omega) \supset U(\Omega) \otimes U_{ST}(4)$$

into the spatial $U(\Omega)$ and spin-isospin $U_{ST}(4)$ branches which are complementary [7]. The chain at the right-hand side of it:

$$SU_{ST}(4) \supset SU_S(2) \otimes SU_T(2)$$

of the Wigner's supermultiplet model [10] gives the spin S and isospin T of the basis states of the shell model. In parallel to it, on the left-hand side we show the two possible reductions of the spatial part $U(\Omega)$ to the SO(3) algebra of the angular momentum. The middle chain [2]

$$U(\Omega) \supset SU(3) \supset SO_L(3)$$

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defines the rotational limit of the model with only quadrupole-quadrupole interaction taken into account. The one on the left – through $SO(\Omega)$ whose representations are equivalent to the SO(8)-ones which is the algebra of the isoscalar and isovector pairing interaction, defines the pairing limit of the shell-model algebra. Both these chains are complementary to the spin-isospin $U_{ST}(4)$ algebra. So, the important result, established in [9] is that the spatial subalgebra $U(\Omega)$ of the shell-model algebra $U(4\Omega)$ contains two distinct dynamical symmetries defined by the reduction chains: through $SO(\Omega)$ and through SU(3). Consequently, both chains determine full-basis sets and could be expressed through each other. The basis states labeled by the quantum numbers of the representations of the algebras in the SU(3) chain

$$|\Psi_R\rangle \equiv |\{f\}\alpha(\lambda,\mu)KL,S;JM\rangle$$

are eigenstates of the rotational limit of the model with quadrupole-quadrupole interaction. Correspondingly, the basis states in which the pairing interaction is diagonal [11] are labeled as:

$$|\Psi_P\rangle \equiv |\{f\}\nu[p_1, p_2, p_3]\beta L, S; JM\rangle.$$

In both types of states α , β and K give the multiplicity labels of the corresponding reductions. Since the microscopic SU(3) model based on the threedimensional harmonic oscillator has a well-developed theory, including the Wigner-Racah algebra for the calculation of matrix elements [12] in the SU(3) basis and various successful applications in real nuclei, we choose to expand the states of the pairing basis $|\Psi_P\rangle$ in the set of basis states $|\Psi_R\rangle$, i.e.

$$|\Psi_P\rangle_i = \sum_j C_{ij} |\Psi_R\rangle_j.$$
⁽²⁾

Using the above expansion and the diagonalization procedure for the pairing interaction in the SU(3) basis:

$${}_{i}\langle\Psi_{P}|H_{Pair}|\Psi_{P}\rangle_{i} = E_{Pair}(m, i, [P], (ST)) = \sum_{jk} C_{ki}^{*}C_{ij}.\delta_{kj}._{k}\langle\Psi_{R}|H_{Pair}|\Psi_{R}\rangle_{j}$$
(3)

we obtain numerically the probability $|C_{ij}|^2$ with which the states of the SU(3) basis enter into the expansion of the pairing basis. In this way we actually calculate the transformation brackets between the two chains [13], which is of great use when calculating the matrix elements of different operators in each of the chains. This is important for example for the calculation of transition probabilities. Also, this expansion could help evaluate the importance (weight) of the different SU(3) states, when we need to impose restrictions on the basis because of computational difficulties. The known relations of the SU(3) labels (λ, μ) and the β, γ shape variables of the geometrical model can be used for the analysis of

Table 1. T the reduction	he classificat on scheme (1	ion of the sta ¹).	tes of 2 particle	es (a) in the l	o shell (Σ	l = 3, (b) ds s	hell ($\Omega = 6$)	and $(c) fp$ she	Il ($\Omega = 10$) according to
(<i>a</i>)	U(3)	SO(3)	$SO_p(3)$	SU(3)		$SO_L(3)$	$U_{ST}(4)$	$SO_P(6)$	$SU_S(2) imes SU_T(2)$
1	$\{\tilde{f}\}$	$[\mu]$	$\nu[p]$	(λ,μ)	Κ	T	$\{f\}$	[P]	(ST)
	$\{1^2\}_3$	$[1^{2}]_{3}$	2[1]	$(0, 1)_{3}$	0	1	$\{2\}_{10}$	$[1^3]_{10}$	$(0,0)_1 \\ (1,1)_9$
I	$\{2\}_6$	$[0]_{1}$	0[0] $2[1^3]$	$(2,0)_6$	0	0, 2	$\{1^{2}\}_{6}$	$[1]_{6}$	$(1,0)_3$ $(0,1)_3$
I									
= (q)	$U(\tilde{6})$	SO(6)	$SO_p(6)$	SU(3)	;	$SO_{L}(3)$	$U_{ST}(4)$	$SO_P(6)$	$SU_S(2) imes SU_T(2)$
I	$\{f\}$	$[\mu]$	$\nu[p]$	(λ,μ)	Κ	L	$\{f\}$	[P]	(ST)
	$\{1^2\}_{15}$	$[1^2]_{15}$	2[1]	$(2,1)_{15}$	1	1, 2, 3	$\{2\}_{10}$	$[1^3]_{10}$	$(0,0)_1 \ (1,1)_9$
I	$\{2\}_{21}$	$[0]_{1}$	0[0]	$(4,0)_{15}$	0	0, 2, 4	$\{1^2\}_6$	$[1]_6$	$(1, 0)_{3}$
1		$[2]_{20}$	$2[1^3]$	$(0,2)_{6}$	0	0, 2			$(0, 1)_3$
=	17/10)	01/02	CO (10)	CI1/9)		(6) - OS	11(A)	$(\theta) = (\theta)$	
(c)	U(10) $\{\tilde{f}\}$	(01) [μ]	$\nu[p]$	(λ, μ)	Κ	$(e)^T O C$	$UST(4)$ $\{f\}$	P[P]	$SUS(z) \times SUT(z)$ (ST)
	$\{1^2\}_{45}$	$[1^2]_{45}$	2[1]	$(4,1)_{35} \ (0,3)_{10}$	1 0	$1,2,3,4,5\\1,3$	$\{2\}_{10}$	$[1^3]_{10}$	$(0,0)_1 \ (1,1)_9$
I	$\{2\}_{55}$	$[0]_1$	$0[0] 2[1^3]$	$(6,0)_{28}$ $(2.2)_{27}$	00	0,2,4,6 $0,2.4$	$\{1^2\}_6$	$[1]_{6}$	$(1,0)_3$ $(0,1)_3$
			- - -		5	2, 3			

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Figure 1. SU(3) contents of the lowest pairing eigenstate for the system of 2 (left) and 4 (right) identical particles in the $f_{7/2}$ orbital ($\Omega = 8$).

the deformations of the pairing states, expressed through the respective SU(3) ones.

The classification of the states of 2 particles in the p shell ($\Omega = 3$), ds shell ($\Omega = 6$) and fp shell ($\Omega = 10$) according to the reduction scheme (1) is presented in Table 1 (the more complicated case for 4 particles has already been illustrated in [9]). It is clear that for each pairing eigenstate only part of the SU(3) representations are involved. Specifically, the lowest pairing eigenstate of seniority $\nu = 0$ is composed of the SU(3) irreps (2,0) in the p shell, (4,0) and (0,2) in the ds shell, and (6,0) and (2,2) in the fp shell.

Next, we present the results for the pairing eigenstates of systems in a single orbital, namely, the $f_{7/2}$ orbital. Energetically, this orbital lies above the orbitals from the ds shell yet still well below the rest of the other orbitals which compose the fp shell. This is the reason 28 to be considered as "magic" number in some shell-model applications. Since we use the expansion (2), from the comparison of the results for 2 and 4 identical particles in the $f_{7/2}$ orbital ($\Omega = 8$), one can see that more SU(3) irreps are involved in the second case, but their contributions diminish (see the right-hand side of Figure 1). Compared to the pairing-in-a-shell eigenstates, we no longer have the restriction of only part of the SU(3) representations to participate in the pairing-in-an-orbital eigenstate which is also illustrated in the figure.

For the purpose of our investigation we use the Hamiltonian:

$$H = H_0 + V_{res} \tag{4}$$

of the PQM [14], where $H_0 = \hbar \omega$ is the harmonic oscillator term or the singleparticle interactions, which we need to introduce when considering the shell plus orbital or the two-shell cases in order to place correctly the single-particle configurations in respect to each other. This introduces one more parameter in this generalization of the model, which influences the applications to real nuclear

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systems, where it will be used. The residual interaction is used in the form:

$$V_{res} = \frac{1}{2}(1-x)\mathbf{G}(S_{\mu}^{\dagger}.S_{\mu} + P_{\mu}^{\dagger}.P_{\mu}) - \frac{1}{2}(1+x)\chi Q.Q,$$
(5)

where obviosly at x = -1 we have pure pairing interaction with equal strengths of the isoscalar and isovector terms and at x = 1 the limiting case of pure quadrupole interaction is realized. At x = 0 we have both interactions mixed with their respective strengths. This allows us to investigate the influence of these residual interactions on the spectra in real nuclear systems.

3 Results and Discussion

After presenting in short the algebraic realization of the dynamical symmetries that appear in the microscopic shell model we would now like to exploit their applications in realistic nuclear systems. We start with a real test case for the applications of the theory – the ds shell, which is the first one, where both deformation and pairing phenomena play an important role [15], [16]. Our proof-of-case example presents the simple but complete system of 4 particles in the ds shell which allows us to study the PQM without any truncation of the model space. In the same truncation-free environment we are also able to describe the effect on the results, of adding the next fp shell or just its lowest-lying $f_{7/2}$ orbital.

3.1 Results in one shell

On the upper side of Figure 2 we present the results of a minimization procedure for the RMS value $\sigma = \sqrt{\sum_i (E_{Th}^i - E_{Exp}^i)^2/d}$ (per degree of freedom d) with respect to the two parameters G and χ of the residual interaction (5) taken for two different choices of the model space: a single ds shell (top row, lefthand side) and ds + fp shell with $\hbar \omega = 2$ MeV (top row, right-hand side). The black areas in the middle of these figures present the intervals of change of the parameters for which we have the minimal values of σ or the values of the parameters fitted to a set of experimental energies E_{Exp}^{i} from the observed spectra of a real nuclear system. In the presented case we use the energies of the low-lying states of ²⁰Ne, which has 2 protons and 2 neutrons in the ds valence shell. The red dotted line connects the values of each of the parameters G and χ at their respective limiting cases of pure pairing or pure quadrupole-quadrupole interactions. This line could be assigned as the axis of change of the parameter $-1 \le x \le 1$ defined in (5) and used. The regions of the optimal values for the parameters lie on this line and their position in respect to its center could serve as a measure of the influence of each of the terms of the residual interaction on the energy spectra of the considered nucleus.





Figure 2. Description of the excitation spectrum for the case of 2 protons and 2 neutrons in: upper row left-hand side – only ds single shell and upper row right-hand side – the ds + fp shell calculated in full SU(3) basis using the PQM plus the single-particle interaction at $\hbar\omega = 2$ MeV. Lower panel: comparison of the experimental and theoretical results for the excitation spectrum of ²⁰Ne, calculated in one and two oscillator shells. The values of the Hamiltonian parameters of the best results are given in the figure.

3.2 Results in two shells

Next, for the same system, we extend our investigation beyond one oscillator shell. This way, we can demonstrate how the description of the energy spectrum improves and to what degree the two-shell eigenfunction can be described by its one-shell restriction. The addition of $f_{7/2}$ or the whole fp shell to the model space is expected to improve the one-shell results.

The addition of the single-particle term to the Hamiltonian accounts for the separation of the orbits in the two adjacent shells. At the right-hand side of the upper row in Figure 2 we show the improvement of adding the fp shell to the model space where the $f_{7/2}$ orbital has the same energy as the rest of the orbitals from the fp shell. It was demonstrated in [17] that the single-particle strength $\hbar\omega$ determines at which value of χ the dominant SU(3) irrep will change from

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Figure 3. The overlap of the eigenstate, obtained in the two-shell model space $(|\Psi_0\rangle, |\Psi_1\rangle)$, with the result in the single ds shell $|\xi_0\rangle$ and ds plus the $f_{7/2}$ orbital as an intruder $|\xi_1\rangle$ for the system of 2 protons and 2 neutrons in the dsfp shell at G = 0.2 MeV and varying values of the parameter χ . In the $|\Psi_0\rangle$ eigenfunction, the $f_{7/2}$ orbit is considered energetically to belong to the ds shell. In the $|\Psi_1\rangle$ case, $f_{7/2}$ belongs to the fp shell. Results are shown for (a) $\hbar\omega = 10$ and (b) 20 MeV, respectively.

(8,0) (the leading representation with zero particles in the fp shell) to (12,0) (the one with four particles in the fp shell). It was also established that the pairing interaction can only smooth down this transition without interfering at which point it occurs. At the lower panel of Figure 2 it is shown that in the excitation spectrum of ²⁰Ne the degeneracy of the second and third J = 0 and J = 2 states is removed and these levels exactly reproduce the ordering of the collective states of the experimental spectrum. Also, the RMS value σ shows improvement – it is reduced from 0.83 to 0.69 MeV. Further upgrade of the result can be achieved if the $f_{7/2}$ orbital is considered as an orbit separated from the remaining part of the fp shell.

Finally, in Figure 3 we demonstrate that the two-shell results $|\Psi_0\rangle$, $|\Psi_1\rangle$ can be quite well represented at certain interaction strengths by the eigenfunctions in only one shell $|\xi_0\rangle$ or the shell plus a single orbital configuration $|\xi_1\rangle$. The strongest overlap, almost independent of the interaction strengths, is obtained for the case $\langle \Psi_1 | \xi_0 \rangle$, followed by the $\langle \Psi_0 | \xi_1 \rangle$, which starts to diminish at higher values of χ . The fall down of the green curve with rising χ on the left part of the figure can easily be explained by the appearing dominance of the (12,0) representation, a description which goes beyond the one-shell consideration. This effect is missing on the right-hand side of the figure, since with the increase of the $\hbar\omega$ values the change of the dominance is moved towards bigger χ values. A similar effect can be seen with the red curve which point to structure differences between the two-shell and the shell plus an orbital eigenstate. Finally, such an effect is missing on the blue curve for these χ values.

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4 Conclusions

On the basis of the algebraic reductions of the shell-model algebra $U(4\Omega)$ through the dynamical symmetries defined by the pairing algebra SO(8) and Elliott's SU(3) algebra, we explore the relation between the two bases and elucidate the algebraic structure of an extended Pairing-plus-Quadrupole Model, in the framework of the SU(3) scheme [7]. This allows us to study the complementarity and competitive effects of the quadrupole-quadrupole and pairing interactions on the energy spectra of the nuclear systems.

In this paper, we extended the investigation of these effects in a single shell to the consideration of a shell plus an orbital and two-shell cases which are both contained in the employed algebraic approach. This leads to the use of richer model spaces and to a generalization of the PQM that includes a singleparticle interaction, which defines the spacing between the considered shells. Applications of the theory are used as a test of principle for a realistic nuclear system of two protons and two neutrons in the ds shell and the ds + fp shell. The theoretical results are compared with experimental energy spectrum of the ²⁰Ne nucleus, from where the optimal values of the parameters of the residual interactions G and χ are obtained. In the two-shell case this is investigated for different values of $\hbar\omega$ and the best result for σ is presented. A more accurate description of the interplay between the PQM's interactions would require a three-parameter fit to the experiment. Nevertheless, even in this simplified case the obtained results are improved compared to the single-shell case, by lifting the degeneracy in the theoretical collective levels and reproducing their ordering.

We also investigate the possibility of approximating the two-shell results with the single shell and the single-shell plus orbital ones, which could be very useful in studying the role of the intruder orbital in heavier shells. This investigation traces the way to the more elaborated and accurate predictions of the collective properties of nuclei, where protons and neutrons fill the same shell, which are of utmost importance for the nuclear astrophysics.

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