Isovectorial pairing in solvable and algebraic models

Sergio Lerma¹, Carlos E Vargas¹ and Jorge G Hirsch²

¹ Departamento de Física, Facultad de Física e Inteligencia Artificial, Universidad Veracruzana, Lomas del Estadio s/n, C.P. 91000, Xalapa, Veracruz, México
² Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, AP 70-543, 04510 Mexico DF, Mexico
E-mail: slerma@uv.mx

Abstract. Schematic interactions are useful to gain some insight in the behavior of very complicated systems such as the atomic nuclei. Prototypical examples are, in this context, the pairing interaction and the quadrupole interaction of the Elliot model. In this contribution the interplay between isovectorial pairing, spin-orbit, and quadrupole terms in a harmonic oscillator shell (the so-called pairing-plus-quadrupole model) is studied by algebraic methods. The ability of this model to provide a realistic description of N=Z even-even nuclei in the fp-shell is illustrated with ⁴⁴Ti. Our calculations which derive from schematic and simple terms confirm earlier conclusions obtained by using realistic interactions: the SU(3) symmetry of the quadrupole term is broken mainly by the spin-orbit term, but the energies depends strongly on pairing.

1. Introduction

Starting from a harmonic mean field and a spin-orbit one-body term, the independent particle shell model of atomic nuclei is able to reproduce the shell closures found experimentally and to describe dominant features of closed shell nuclei. When the number of nucleons deviates from the magic numbers, residual interactions have to be taken into account for a proper description of these nuclei. Two dominant terms of these residual forces are the quadrupole and pairing interactions [1]. A common characteristic of these two-body interactions is that they can be approximated by schematic terms possessing an underlying algebraic structure which can be exploited to simplify their study and to interpret clearer their effects. The pairing plus quadrupole Hamiltonian of Bohr, Mottelson and Belyaev [2, 3] is obtained by bringing together all the previous terms and by supposing a valence space by only one harmonic oscillator shell:

\[ H = C \sum_i l_i \cdot s_i - \frac{\chi}{2} Q \cdot Q + H_p. \]  

The relevance of the different terms in Hamiltonian (1) to describe nuclei in the sd and pf shells has been the subject of several studies, which make use of realistic interactions to derive their results. In ref. [4] the authors showed that the spin-orbit and quadrupole deformation terms suffice to give a correct description of the wave functions for systems with 4 protons and 4 neutrons in the pf, sdq and pfh shells. Additional terms in the Hamiltonian (pairing terms included) change the spectrum without modifying strongly the wave functions. Similar results were reported in [5] for different nuclei in the lower pf shell, there it was found that the spin-orbit
splitting is responsible for the breaking of the SU(3) symmetry associated to the quadrupole interaction, and that this breaking has a small influence in the B(E2) transition probabilities, which remain close to the values coming from exact SU(3) calculations. The latter result is a consequence of what has been called quasi SU(3) dynamical symmetry or adiabatic mixing of SU(3) irreps [6, 7]. The role of the different pairing channels was discussed in ref. [8]. In this reference it is shown, in the framework of full pf shell model calculations with a realistic KB3 interaction, that the proton-neutron components of pairing are very relevant to correctly describe the moment of inertia of $^{48}$Cr nuclear rotors, a conclusion already signaled in ref. [9], where the authors concluded that the failure of the HFB method to describe the moment of inertia of $^{48}$Cr can be attributed to an improper treatment of pairing correlations. Even if the previous results are very illustrative and robust, it is desirable to have a framework where they can be understood in simpler terms. The present work goes in that direction by considering a simple Hamiltonian with the minimal ingredients for a realistic description of atomic nuclei.

The interplay between the different terms in Hamiltonian (1) has been studied in refs. [10, 11]. In the first of these, the pairing interaction is shown to induce soft triaxial deformations in, otherwise, SU(3) symmetric nuclei with sharp oblate or prolate deformations. It is worth to mention that the previous works included only a kind of nucleon, consequently only the like particle component of the isovectorial pairing interaction is taken into account. The role of the spin-orbit term in the Elliot model is analyzed in ref. [12]. The authors take into account the isospin degree of freedom (but no pairing terms) to suggest a SU(3)-based truncation procedure to diagonalize Hamiltonians in large spaces.

Two works closely related to the present one can be found in [13, 14]. In the former the isovectorial pairing without proton-neutron component and the spin-orbit term are introduced in the Elliot model. The SU(3) truncation procedure previously mentioned is used to describe the yrast energies of $^{48}$Cr. Although the energies obtained in this reference do not reproduce the experimental backbending of $^{48}$Cr, the structure of the wave functions in terms of SU(3) irreps presents a change in the yrast states where backbending happens. The authors conclude that the lack of proton-neutron pairing correlations may explain the absence of backbending in the spectrum of the model, a conclusion that is supported by the results given in reference [14], where the role of the different pairing channels is studied by using the same Hamiltonian as eq.(1). In particular it is found that the isovectorial pairing is at the origin of the backbending of $^{48}$Cr.

In this contribution all the components of isovectorial pairing are included in addition to the spin-orbit and quadrupole terms in the framework of the Elliot model, i.e., by using a SU(3) basis. The breaking of the SU(3) symmetry by the spin-orbit and pairing terms is studied. The model is employed to describe the yrast states of the (N=Z) $^{44}$Ti nucleus. In Section 2 the symmetric limits of the model are briefly discussed, whereas in Section 3 the exact solution of the isovectorial pairing with arbitrary single-particle energies (spin-orbit term in this context) is reviewed. The method used to diagonalize the Hamiltonian in a SU(3) basis is presented in Section 4. Results and some conclusions are given in Sections 5 and 6 respectively.

2. The symmetric limits
A good description of light rotational nuclei in the sd-shell is provided by the Elliot model [15]. This model assumes a single shell of the spherical harmonic mean field ($\eta$) and a quadrupole-quadrupole residual interaction

$$H_Q = -\frac{\chi}{2} \mathbf{Q} \cdot \mathbf{Q},$$

which can be expressed as a linear combination of the Casimir operators of the group chain [16] $SU(3) \supset SO(3)$: $\mathbf{Q} \cdot \mathbf{Q} = 4C_2[SU(3)] - 3C_2[SU(3)]$, where $Q_\mu = \sum_\lambda \sqrt{8(2l + 1)} a_{l\sigma}^{\dagger} \bar{a}_{\sigma \tau}^{(200)}$, with $a_{l\sigma}^{\dagger}$ nucleon creators of angular momentum, spin and isospin $l, \sigma$, and $\tau$, $\bar{a}$ is the
tensorial respective nucleon annihilator, and the sum runs over \( l = \eta, \eta - 2, \ldots, 0 \) or 1. In the coupled operator, the superindex (200) refers to the total orbital angular momentum, the total spin and the total isospin, while the subindex \((\mu 0 0)\) describes their projections.

On the other hand, the pairing interaction that explains naturally the even-odd staggering of nuclear masses and the gap energy in the spectrum of even-even nuclei, can be modeled by the schematic interaction

\[
H_p = -g_1 \mathbf{b}^\dagger \cdot \mathbf{b} - g_0 \mathbf{D}^\dagger \cdot \mathbf{D},
\]

where the dots represent scalar couplings in isospin and spin space respectively. The isovectorial and isoscalar pairs, written in a \( ls \) scheme, are

\[
b^\dagger_{t_z} = \sum_l \sqrt{\frac{2l+1}{2}} \left[ a^\dagger_{l\sigma, \tau} \times a^\dagger_{l\bar{\sigma}, \bar{\tau}} \right]^{(01)}_{(00, l_\sigma, l_\tau)} , \quad D^\dagger_{s_z} = \sum_l \sqrt{\frac{2l+1}{2}} \left[ a^\dagger_{l\sigma, \tau} \times a^\dagger_{l\bar{\sigma}, \bar{\tau}} \right]^{(01)}_{(00, l_\sigma, l_\tau)}.
\]

The isovectorial pairing interaction above, includes the like particles pairing (\( b^\dagger_{t_z} \) with \( t_z = -1 \) and \( t_z = 0 \)), and the two channels of proton-neutron pairing (\( b^\dagger_{t_z=0} \) and \( D^\dagger_{s_z} \)).

It can be shown [17] that the pair creators are the ladder operators of a SO(8) algebra. If \( g_1 = g_0 \), the pairing Hamiltonian can be expressed in terms of the Casimir operator of that algebra and the model commutes with the generators of the SU(4)-Wigner symmetry. In the case where only isovectorial or isoscalar channels are included, the pairing interaction can be expressed in term of the Casimir operator of a SO(5) algebra, and the model is, respectively, isospin or spin invariant. In all of the previous symmetric cases, the wave function of the ground state for \( N = Z \) even-even systems exhibits a quartet structure in the symmetric space. If only one kind of nucleons is allowed, a situation that arise when the valence protons and valence neutrons occupy different shells, the relevant algebra is reduced to the more tractable SU(2) algebra.

The most general case \((g_1 \neq g_0)\) has been studied in [18], where it is shown that the quartet structure of the ground state wave function found in the symmetric limits, remains in the following form

\[
\left( \cos \theta \mathbf{b}^\dagger \cdot \mathbf{b}^\dagger - \sin \theta \mathbf{D}^\dagger \cdot \mathbf{D}^\dagger \right)^{(M/2)} |0\rangle.
\]

where \( \theta \) is a parameter which takes the values \( \theta = 0 \) for pure isovectorial pairing, \( \theta = \pi/2 \) for pure isoscalar pairing and \( \theta = \pi/4 \) for \( g_1 = g_0 \).

Before discussing the solution for a Hamiltonian which additionally includes a spin-orbit term, it is convenient to mention the work of ref. [19], where it is shown that the spin-orbit is very effective to suppress the isoscalar correlations, leaving the isovectorial ones unaffected. This result that can be understood by expressing the isovectorial and isoscalar pairs in a \( jj \)-scheme, while the isovectorial pairs relates nucleons in the same \( j- \) shell, the isoscalar pairs are formed by nucleons in different \( j \)-shells. For that reason, in what follows only the isovectorial pairing will be considered.

3. Exact solution of the isovectorial pairing plus spin-orbit interaction

The isovectorial pairing with the spin-orbit term is a particular case of the isovectorial pairing Hamiltonian with arbitrary single-particle energies,

\[
H_{SO(5)} = \sum_i \epsilon_i \left( N_{pi} + N_{ni} \right) - g \sum_{ij} \left( b^\dagger_{i1} b_{ij} + b^\dagger_{i0} b_{ij} + b^\dagger_{-1j} b_{ij} \right),
\]

which has been shown to be diagonalizable by a Bethe ansatz in refs.[20, 21]. The energies of the previous Hamiltonian are given by \( E = \sum e_s \), where the parameters \( e_s \) are the solution of
the following set of non-linear equations which involves additionally a set of parameters \( \omega_p \):

\[
\sum_{q \neq s}^M \frac{2}{e_s - e_q} + \sum_q^M \frac{1}{\omega_q - e_s} + \sum_j \frac{1}{2\epsilon_j - e_s} = \frac{1}{g}, \quad \sum_q^M \frac{2}{e_q - \omega_p} + \sum_{q \neq p}^M \frac{2}{\omega_p - \omega_q} = 0,
\]

with \( s = 1, \ldots, M \) and \( q = 1, \ldots, M - T \), where \( M \) and \( T \) are, respectively, the number of pairs and isospin of the eigenstate.

Besides the energy, the parameters \( e_s \) determine the orbital and spin structure of the correlated pairs through

\[
b^\dagger_i(e) = \sum_{i} \frac{b^\dagger_{ti}}{2\epsilon_t - e},
\]

whereas the \( \omega_q \) parameters determine the wave function structure in isospin space. General expression can be found in [22]. Here we only signal that, for the simplest non-trivial case of \( N = Z = 4 = M \), it was shown that the wave function can be approximated by

\[
\left. \left(b^\dagger(e_1) \cdot b^\dagger(e_2) \right) \left(b^\dagger(e_3) \cdot b^\dagger(e_4) \right) \right| 0, \]

for almost all values of the pairing strength, except for small ranges around the values where one pair changes its orbital character from a normal pair (uncorrelated pairs occupying the single-particle levels) to a Cooper-like pair. The previous expression is reminiscent of the quartet structure found in the case of one completely degenerate shell, eq.(2), but contrary to that case, here the quartets are not identical. Only in the limit \( g \to \infty \) (which implies \( |e_s| \to \infty \)), the effect of the single-particle energies is diluted and the one-shell solution is recovered.

One of the advantages of the Bethe ansatz is that it can be used to explore the solution in very large spaces, where standard diagonalization techniques are unable to manage the problem. As an illustration of this, in figure 1 a graphical representation of the solution is shown for the case of 44 nucleons (\( N = Z = 22 \)) moving in a set of single particle energies given by the first six harmonic oscillator shells (\( \eta = 0, \ldots, 5 \)) and a spin-orbit term. The figure shows two cases, the first one, corresponding to weak paring strength where all the pairs are associated to the lowest single-particle levels, represents the case of uncorrelated pairs formed by nucleons occupying the single-particle levels. In the second case, only the deepest pairs remain associated to the single particle levels, the pairs in the upper part expand in the complex plain, signaling the formation of a superconducting state whose structure in isospin space is very difficult to determine.

4. Isovectorial pairing interaction in a SU(3) basis

The quadrupole term breaks the exact solvability of the pairing plus spin-orbit Hamiltonian, therefore a different procedure is needed. The results of refs.[4, 5] indicates the most convenient way to proceed: rather than including the quadrupole as a perturbation in the previous exact solution, it is better to include the previous Hamiltonian in a basis which diagonalizes the quadrupole-quadrupole term. This basis is given by the following chain of groups [12, 23]:

\[
\begin{align*}
[1^N] \quad \left[ f_{\tau} \right] \quad [f_{\tau}] \quad \alpha_{\tau} \quad (\lambda_\tau, \mu_\tau)s_\tau
\end{align*}
\]

\[
U(\Omega_\tau) \supset U \left( \frac{\Omega_\tau}{2} \right) \times U(2) \supset SU(3) \times SU(2),
\]

where \( \tau = p, n \) and \( \Omega_\tau \) is the degeneracy of the harmonic oscillator shell. The previous classification applies to protons and neutrons separately, the basis we use is obtained by coupling the proton and neutron SU(3) irreps to a total SU(3) irrep:

\[
\left| \{ N_p[f_p]\alpha_p(\lambda_p, \mu_p)s_p \} \left\{ N_n[f_n]\alpha_n(\lambda_n, \mu_n)s_n \right\} \rho(\lambda, \mu)\kappa LS ; JM \right>,
\]
where $\rho$ and $\kappa$ are multiplicity labels which count respectively, the number of times the irrep $(\lambda, \mu)$ occurs in the product $(\lambda_p, \mu_p) \otimes (\lambda_n, \mu_n)$ and the number of occurrences of the angular momentum $L$ in the irrep $(\lambda, \mu)$.

To calculate the matrix elements of the Hamiltonian in the previous basis, we need to express the pairing and spin-orbit terms as a linear combination of $SU(3)$ tensors. With these expressions and eq. (10) of ref.[23], which derives directly from the Wigner-Eckart theorem, the matrix elements are expressed in terms of reduced matrix elements, which, in turn, can be calculated employing the code described in ref.[24]. The expression for the spin-orbit and like particles pairing can be found in refs.[12, 23], the only term that remains to be calculated is the proton-neutron component of isovectorial pairing. The result is given here

$$H_{PN} = \frac{g}{2} \sum_{\lambda_p, \lambda_n} \sum_{\lambda_o, \mu_o} \sum_{\rho_o} \sqrt{2s + 1} C(\lambda_p, \lambda_n, \lambda_o, \mu_o, \rho_o) \left[ \tilde{a}_{p(\eta,0)}^{(\lambda_p,\lambda_p)^s} \right] \left[ \tilde{a}_{n(0,\eta)}^{(\lambda_n,\lambda_n)^s} \right] \rho_o(\lambda_o, \mu_o, \kappa_o = 1 \to 0, s_o = 0), \quad (4)$$

where the function $C$ is given by $SU(3)$ Clebsch-Gordan coefficients

$$C(\lambda_p, \lambda_n, \lambda_o, \mu_o, \rho_o) = \sum_{L, L'} \sum_{\kappa_p, \kappa_n} \sqrt{2L + 1} \langle \lambda_p, \mu_p | l(0, \eta) l' | \lambda_n, \mu_n \rangle \times \langle \lambda_p, \mu_p | \kappa_p, \kappa_n, L \rangle \times \langle \lambda_n, \mu_n | L \rangle \times \langle \lambda_o, \mu_o \rangle_{\kappa_o = 1 \to 0, s_o = 0}. \quad (5)$$

5. Results for $^{44}$Ti
The strength ratios of the different forces in the Hamiltonian are fixed by systematics [1, 25]:

$$\frac{C}{\epsilon_o} = \frac{2}{\hbar \omega_o \kappa} \approx \frac{0.16}{A^{1/4}} \left[ MeV \right], \quad \frac{x}{\epsilon_o} = \frac{28}{A^{5/3}} \left[ MeV \right], \quad \frac{g}{\epsilon_o} = 19.51/A \left[ MeV \right].$$

where the parameter $\epsilon_o$ is a dimensionless, global parameter that only fix the energy scale without modifying the wave functions.
Figure 2. Yrast spectrum of $^{44}$Ti, the first column shows the experimental values, the last three columns are obtained from the model Hamiltonian with all (2nd column), quadrupole+spin-orbit (3rd column), and quadrupole+pairing (4th column) terms.

We use a system corresponding to $^{44}$Ti to illustrate our results. This system contains two valence protons and two valence neutrons moving in the $\eta = 3$ oscillator shell, where the spin orbit-term produces 4 single particle-levels ($f_{7/2}, p_{3/2}, p_{1/2}, f_{5/2}$). The dimension of the space allows a full diagonalization, however a SU(3) dictated truncation can employed in nuclei with larger spaces. To probe the procedure and the written code, we compare the energies obtained for a Hamiltonian without quadrupole term with the energies coming from the exact solution for $\epsilon_o = 1$. Results are shown in table 1 for the ground state energy (measured respect to the zero energy of the oscillator) and for the excitation energy of the first seniority two state ($J = 2, 4, 6$). The SU(3) code reproduces perfectly the energies and degeneracies obtained from the exact solution.

In the first and second columns of figure 2, the spectrum of the model is compared with the experimental energies of the yrast states of $^{44}$Ti. The overall parameter $\epsilon_o$ was fixed at 0.7. In the third and fourth columns of the same figure, the spectra of the Hamiltonians without pairing and without spin-orbit term are shown. Note that the quadrupole plus spin-orbit Hamiltonian exhibits a rotational spectrum and that the non-rotational character of $^{44}$Ti spectrum is reproduced by the pairing term. From these results one could naively conclude that pairing is the responsible of the SU(3) symmetry breaking of the quadrupole term, a wrong conclusion which is refuted by the evidences coming from analyzing the respective wave functions.

In figure 3 the contribution of the different SU(3) irreps to the ground state wave functions is shown for the three cases of figure 2. From this figure, it is clear that the SU(3) fragmentation is mainly dictated by the spin-orbit term, whereas the pairing term produces a wave function

| GS energy ($J = 0$) | SU(3) Code | Exact Solution |
|---------------------|------------|---------------|
| $\Delta E_2$ ($J = 2, 4, 6$) | 192.54 MeV | 192.54 MeV |
|                     | 2.3905 MeV | 2.3904 MeV |

Table 1. Comparison between SU(3) code and exact solution results for the ground-state energy and excitation energy of the first seniority two state, for an isovectorial pairing plus spin-orbit Hamiltonian.
dominated completely (80 %) by the SU(3) irrep with largest SU(3) casimir value (which is the ground-state wave function in the pure quadrupole SU(3) symmetric limit). Figures 2 and 3 illustrates the way as the SU(3) symmetry is broken in the case of realistic values of the Hamiltonian parameters: the spin-orbit term is the responsible of the SU(3) breaking even if its influence in the spectrum is rather marginal, on the contrary the pairing term breaks slightly the SU(3) symmetry of the quadrupole term, but the spectrum depends strongly on it. The SU(3) fragmentations of the ground-state wave functions shown in figure 3 are very similar to those obtained in [5] for a realistic Kuo-Brown-3 realistic interaction, which indicates the ability of the model to properly describe real systems despite its simplicity. As the total angular momentum increases, the effect of pairing is reduced due to the Coriolis force which breaks the Cooper pairs. It was verified that the effect of pairing disappears for $J \geq 8$ (seniority four states), a result that can be understood from the fact that these states are obtained by breaking all the pairs of the $f_{7/2}$ subshell, the lowest in energy.

Figure 3. Contribution of the different SU(3) irreps to the ground-state wave functions for the same Hamiltonian as in figure 2. In the horizontal axis the different SU(3) irreps are represented by their Casimir values.

6. Conclusions
Some aspects of isovectorial pairing interaction in the context of an exactly solvable (pairing+spin-orbit) and an algebraic (pairing+quadrupole model) model were discussed. The isovectorial pairing plus spin-orbit term is solvable by a Bethe ansatz, which allows to explore very large systems untractable by other standard methods. The graphical representation of the solution allows a qualitative description of the wave function, but quantitative results are much more challenging. For the simplest non-trivial case ($N = Z = 4$), it was shown that the quartet structure in isospin space found in the model with only one degenerate level, survives the splitting of the single-particle levels for almost all values of the pairing strength. For the Hamiltonian which includes additionally the quadrupole interaction, it was found that, for realistic values of the Hamiltonian parameters, the pairing interaction acts like a “quasi-scalar” tensor, that is to say it breaks slightly the SU(3) symmetry but has a strong effect in the energy spectrum. On the contrary the spin-orbit term determines the way as the SU(3) symmetry of the quadrupole term is broken, but leaves the rotational spectrum of the quadrupole term almost unmodified. The present study can be extended to other $N = Z$ nuclei in the $pf$ shell, in particular to reproduce the experimental backbending of $^{48}$Cr. Work in this direction is underway.
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