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Angular momentum decomposition of Richardson's pairs

G. G. Dussel
Departamento de Física Juan José Giambiagi, Universidad de Buenos Aires and CONICET Ciudad Universitaria, Pabellon 1, 1428 Buenos Aires, Argentina

H. M. Sofia
Departamento de Física, Comisión Nacional de Energía Atómica, and CONICET Avda. del Lbertador 8250, 1429 Buenos Aires, Argentina

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The angular momentum decomposition of pairs obtained using Richardson's exact solution of the pairing Hamiltonian for the deformed ^{174}Yb nucleus are displayed. The probabilities for low angular momenta of the collective pairs are strikingly different from the ones obtained in the BCS ground state.

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I. INTRODUCTION

The concept of elementary modes of excitation originated by Landau [1] has been the basis of a rigorous mathematical treatment of many body problems. This concept was introduced in nuclear physics by Bohr and Mottelson [2] to obtain a unified picture of nuclear structure and later was used in the development of a nuclear field theory [3,4] that used the idea of these elementary excitations as building blocks that conform the states and allow us to understand the nuclear properties. In particular, the mean field description of fermion systems, studied at the beginning of the 1960s, was understood using the Hartree-Fock (HF) approximation, based in the single-particle elementary excitations, or a Hartree-Fock-Bogoliubov approximation (HFB) that has as a ground state a coherent state in terms of pairs. For the pairing interaction this wave function is the BCS one:

$$|BCS\rangle = N \exp(\Gamma^\dagger),$$

where N is a normalization constant and $\Gamma^\dagger$ corresponds to the correlated pair usually called the Cooper pair, that can be written as

$$\Gamma^\dagger = \sum_\alpha \frac{U_\alpha}{V\alpha} c^\dagger_\alpha c^\dagger_{\bar{\alpha}}.$$

In the 1970s [6–8] it has been suggested that the low energy spectrum of even-even nuclei can be explain using as building blocks pairs of fermion coupled to angular momentum zero (S) and two (D). The phenomenological prescription known as an interacting boson model, provides a large variety of collective nuclear states, including states that are spherical, deformed or transitional. Using group theory techniques and a few parameters, in a bosonic Hamiltonian with a quadrupole interaction, to be fixed by the data, the model can describe quite well energy-level systematics for very different types of nuclei. Microscopic approaches to the IBM have been attempted, where the interpretation of the bosons has been done using coherent pairs of particles coupled to angular momentum S or D, where the pairing interaction is responsible for the coupling of the particles [9–11]. A link with the usual geometric quadrupole model has been provided by the introduction of boson intrinsic states defined in terms of a set of parameters directly related to the deformation parameters of the geometrical model [12]. This approach shows that the ground states of deformed nuclei can be considered as a condensate of bosons with angular momentum not well defined. However the projection on well-defined angular momentum states shows that the S and D bosons take care of a big percentage of the wave function of the nuclear ground state [13]. On the other hand, some publications claim that higher angular momentum bosons should be included in order to obtain reasonable parameters and good results for different observables as electromagnetic transitions or one and two particle transfers [14]. In a more recent publication it was proposed that an exact solvable boson Hamiltonian with a repulsive pairing interaction to simulate the influence of the Pauli principle. From the solutions of this Hamiltonian, the spectra of the ground state rotational band [15] was obtained. In this case it was shown that in order to obtain reasonable results, higher angular momenta must be included in the treatment.

Most of the theoretical arguments are based in different approximations that solve the pairing interaction. However, exact solutions of the pairing hamiltonian are available from the 1960s [17]. Even the great importance of these exactly soluble Hamiltonians, for many body systems, went unnoticed for quite a long time up to the moment that some publications of Dukelsky *et al.* [19–22] appeared which follow these lines and applied them to several important cases that include fermion and boson systems. Using the Richardson prescription, it is possible to solve exactly the pairing Hamiltonian starting from a set of single particle states obtained from a mean field approximation. The ground state solution is composed of pairs of particles with a well-defined structure. With this exact solution we can study the angular momentum distribution of the Richardson pairs in different kind of nuclei, going from spherical to deformed ones, in order to clarify two important items:

(i) If pairs of particles coupled to angular momenta S and D are enough to describe the ground state of nuclear systems.
(ii) How similar is the exact ground state to the BCS one for different kind of nuclei.

II. HAMILTONIAN USED AND ITS TREATMENT

We will use a Nilsson Hamiltonian for the single particle energies and to this Hamiltonian we add a pairing interaction:

$$H = \sum_{i,m_i} \epsilon_{i,m_i} \; c^{\dagger}_{i,m_i} c_{i,\bar{m}_i} - \frac{G}{4} \sum_{i,m_i,k,m_k} c^{\dagger}_{i,m_i} c^{\dagger}_{i,\bar{m}_i} \; c_{k,\bar{m}_k} c_{k,m_k}, \quad (1)$$

where the operators $c^{\dagger}_{i,m_i}$ are the creators of a single particle in a Nilsson state i, m_i, $c_{i,\bar{m}_i}$ are the time reversal annihilation operators and ϵ_{i,m_i} are the energies of the corresponding Nilsson levels.

This Hamiltonian can be written in terms of new operators that close an SU(2) commutator algebra

$$H = \sum_{i,m_i} \epsilon_{i,m_i} \; \hat{n}_{i,m_i} - \frac{G}{4} \sum_{i,m_i,k,m_k} A^{\dagger}_{i,m_i} \; A_{k,\bar{m}_k}, \qquad (2)$$

where the set of generators of the SU(2) algebra is

$$A^0_{i,m_i} = \frac{1}{2} c^{\dagger}_{i,m_i} c_{i,m_i} - \frac{\Omega_{i,m_i}}{4}, \qquad A^{\dagger}_{i,m_i} = \frac{1}{2} c^{\dagger}_{i,m_i} c^{\dagger}_{i,\bar{m}_i} \;, \quad (3)$$

being $\Omega_{i,m_i} = 2$ the degeneration of the level (i, m_i). This set of operators fulfill the following commutation relations:

$$\begin{aligned} \left[A^0_{i,m_i}, A^{\dagger}_{k,m_k}\right] &= \delta_{i,j}\delta_{m_i,m_j} A^{\dagger}_{i,m_i}, \\ \left[A^0_{i,m_i}, A_{k,m_k}\right] &= -\delta_{i,j}\delta_{m_i,m_j} A_{i,m_i}, \\ \left[A_{i,m_i} A^{\dagger}_{k,m_k}\right] &= -2\delta_{i,j}\delta_{m_i,m_j} A^0_{i,m_i}, \end{aligned} \qquad (4)$$

that close an SU(2) group for each i, m_i. The Hilbert space of M paired particles moving in levels $i, j, k, \ldots, p$ can be classified in terms of the product of groups $\mathrm{SU}(2)_{i,m_i} \times \mathrm{SU}(2)_{k,m_k} \times \mathrm{SU}(2)_{l,m_l} \times \ldots \mathrm{SU}(2) p, m_p$.

A complete set of states, in the Hilbert space, of M paired particles and ν unpaired ones, being the total number of particles $N = 2M + \nu$, can be written as

$$|i, m_i; k, m_k; \ldots . . p, m_p; \nu\rangle = \frac{1}{\sqrt{\mathcal{N}}} A^{\dagger}_{i,m_i} A^{\dagger}_{k,m_k} \ldots . A^{\dagger}_{p,m_p} |\nu\rangle, \qquad (5)$$

where $\mathcal{N}$ is a normalization constant. The possible number of pairs in each level is 1, because they are fermions that fulfill the Pauli principle, and the state ν corresponds to unpaired particles occupying the rest of the states.

Following [20] the pairing interaction corresponds to the rational family of the Richardson-Gaudin (RG) soluble models. In this family, the integrals of motion can be written in terms of the group generators:

$$R_{i,m_i} = A^0_{i,m_i} - 2G \sum_{k,m_k} \left\{ \frac{[A^{\dagger}_{i,m_i} A_{k,m_k} + A_{i,m_i} A^{\dagger}_{k,m_k}]}{2(\epsilon_{i,m_i} - \epsilon_{k,m_k})} + \frac{A^0_{i,m_i} A^0_{k,m_k}}{(\epsilon_{i,m_i} - \epsilon_{k,m_k})} \right\}. \qquad (6)$$

Each of these R_{i,m_i} depends on one parameter, that in the rational mode, is equal to the energy of the level ϵ_{i,m_i} [16]. It can be checked that they commute between themselves and with the operator $A^0 = \sum_{i,m_i} A^0_{i,m_i}$. Following the method first introduced by Richardson [17,18], the eigenvalue problem of these operators $R_{i,m_i}|\Psi\rangle = r_{i,m_i}|\Psi\rangle$ can be solved. The corresponding eigenvectors appear in terms of some collective pair operators.

$$|\Psi\rangle = \prod_{\alpha=1}^{M} B^{\dagger}_{\alpha}|\nu\rangle, \qquad B^{\dagger}_{\alpha} = \sum_j \frac{1}{(E_\alpha - \epsilon_j)} A^{\dagger}_j, \qquad (7)$$

where M is equal to the number of collective $B^{\dagger}$ operators that comprise the state. The structures of the collective operators are determined by a set of M parameters E_α, which satisfy the set of coupled nonlinear equations

$$1 + 2G \sum_{k,m_k} \frac{d_{k,m_k}}{2\epsilon_{k,m_k} - E_\alpha} + 2G \sum_{\beta(\neq\alpha)} \frac{1}{E_\beta - E_\alpha} = 0, \quad (8)$$

where $d_{k,m_k} = \nu_{k,m_k}/2 - \Omega_{k,m_k}/4$ takes care of the degeneracy of the level. The associated eigenvalues take the form

$$r_{i,m_i} = d_{i,m_i} \left\{ 1 - 2G \sum_{k,m_k(\neq i,m_i)} \frac{d_{k,m_k}}{\epsilon_{i,m_i} - \epsilon_{k,m_k}} + 4G \sum_{\alpha} \frac{1}{E_\alpha - 2\epsilon_{i,m_i}} \right\}. \qquad (9)$$

We note here that each independent solution of the set of nonlinear coupled equations (8) defines an eigenstate (9) whose eigenvalues are given by

$$E = 2G \sum_{\alpha} E_\alpha. \qquad (10)$$

From Eq. (1), and making use of Eqs. (8) and (10), a set of M coupled linear equations in terms of M new unknowns can be obtained. The energies E_α solutions of Eq. (9) can be either real or complex conjugate pairs. However, due to the fact that the complex solutions appear always as conjugate pairs, the eigenvalues of the operator R given by Eq. (9) are always reals. Details of the derivation can be found in Refs. [22,23].

The occupation probabilities for the different levels can be obtained from the Hellmann-Feynman theorem, i.e.,

$$n_{i,m_i} = \left\langle \frac{\partial H}{\partial \varepsilon_{i,m_i}} \right\rangle = \sum_{\alpha} \frac{\partial E_\alpha}{\partial \varepsilon_{i,m_i}}. \qquad (11)$$

These occupation probabilities can be used to make an estimation on the value of the gap parameter. If we replace $n_{i,m_i} = V^2_{i,m_i}$ and use the BCS definition of the gap

$$\Delta = G \sum_{i,m_i} U_{i,m_i} V_{i,m_i}, \qquad (12)$$

we can obtain an estimate value of the gap parameter related to the Richardson solution.

III. ANGULAR DISTRIBUTION OF THE RICHARDSON PAIRS

Starting from the solution of the Hamiltonian [Eq. (1)] we have the structure of the different Richardson's pairs in terms

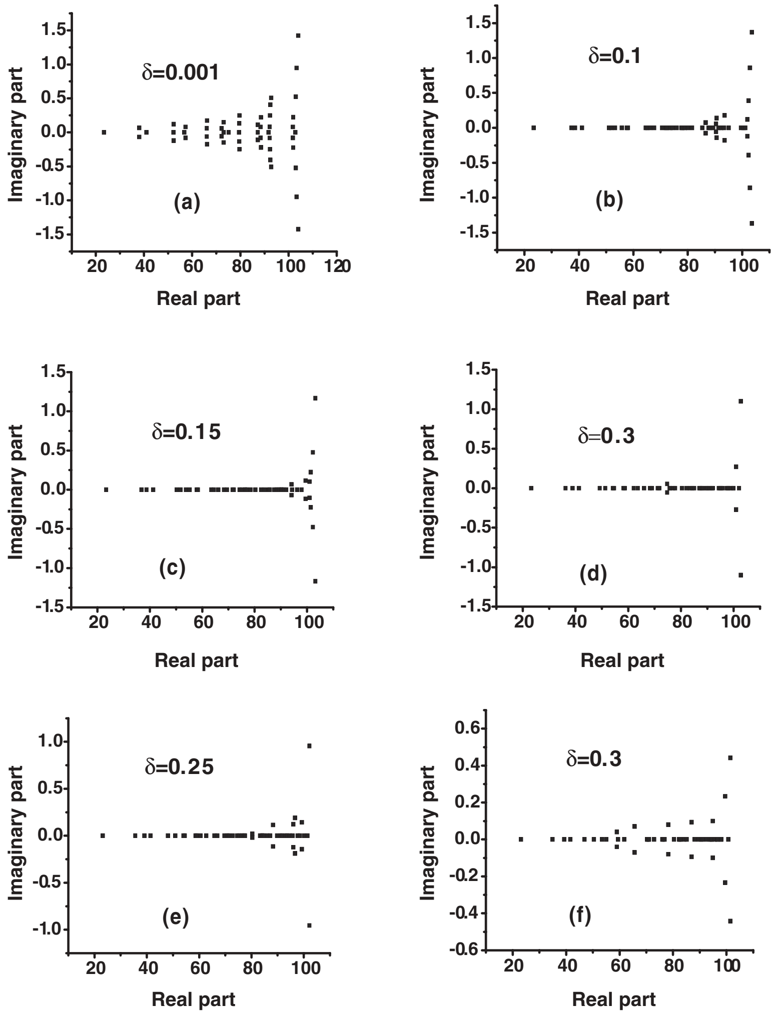

FIG. 1. In this figures are display the imaginary part against the real part of the energy eigenvalues of the Richardson's neutron pairs, for ^{174}Yb. The different figures, from (a) to (f) are the results obtained for increasing values of the deformation parameter δ. Notice that for the pairs with lower energies, the eigenvalues are reals, but the imaginary part, related to the collectivity of the pairs, begins to increase as the energy approach the fermi level.

of the Nilsson-pairs:

$$B_\alpha^+ = \sum_{k,m>0} \lambda_{k,m}^\alpha c_{k,m}^\dagger c_{k,\bar{m}}^+, \tag{13}$$

where

$$\lambda_{k,m}^\alpha = \frac{1}{2\epsilon_{k,m} - E_\alpha}. \tag{14}$$

One thing we are interested in elucidating is the angular momenta composition of the exact solution of a pairing Hamiltonian (1). With this object in mind, we need a representation of the pair B_α in terms of spherical single particle operators with a good angular momentum quantum number. For this, we transform the Nilsson single particle operators in spherical ones using the Nilsson transformation:

$$c_{k,m}^\dagger = \sum_j \Lambda_{j,m}^k b_{j,m}^\dagger, \tag{15}$$

where $b_{j,m}^\dagger$ is the creation operator of a fermion in the state j, m, where j, m are the angular momentum and the magnetic number, respectively. In terms of these spherical operators, the pairs are defined by

$$\begin{aligned} B_\alpha^\dagger &= \sum_{k,m>0} \sum_{j_1,j_2} \lambda_{k,m}^\alpha \Lambda_{j_1,m}^k \Lambda_{j_2,\bar{m}}^k b_{j_1,m}^\dagger b_{j_2,\bar{m}}^\dagger \\ &= \sum_{j_1,j_2,J} a_{j_1,j_2,J}^\alpha [b_{j_1}^\dagger b_{j_2}^\dagger]_0^J. \end{aligned} \tag{16}$$

The coefficient $a_{j_1,j_2,J}^\alpha$ can be easily calculated:

$$\begin{aligned} a_{j_1,j_2,J}^\alpha &= \sum_{k,m>0} \frac{1}{2} \lambda_{k,m}^\alpha \Lambda_{j_1,m}^k \Lambda_{j_2,m}^k \\ &\quad \langle j_1 j_2 m - m | J0 \rangle (-)^{j_2-m} [1 + (-)^J]. \end{aligned} \tag{17}$$

So the pair can be developed as a linear combination of different parts with good angular momentum:

$$B_\alpha^\dagger = \sum_J \sum_{j_1,j_2} a_{j_1,j_2,J}^\alpha \left[b_{j_1}^\dagger b_{j_2}^\dagger\right]_0^J. \tag{18}$$

Therefore, we can see that the relative amount of angular momentum J in the Richardson pair B_α is given by

$$P_J^\alpha = 2 \sum_{j_1,j_2} \left|a_{j_1,j_2,J}^\alpha\right|^2. \tag{19}$$

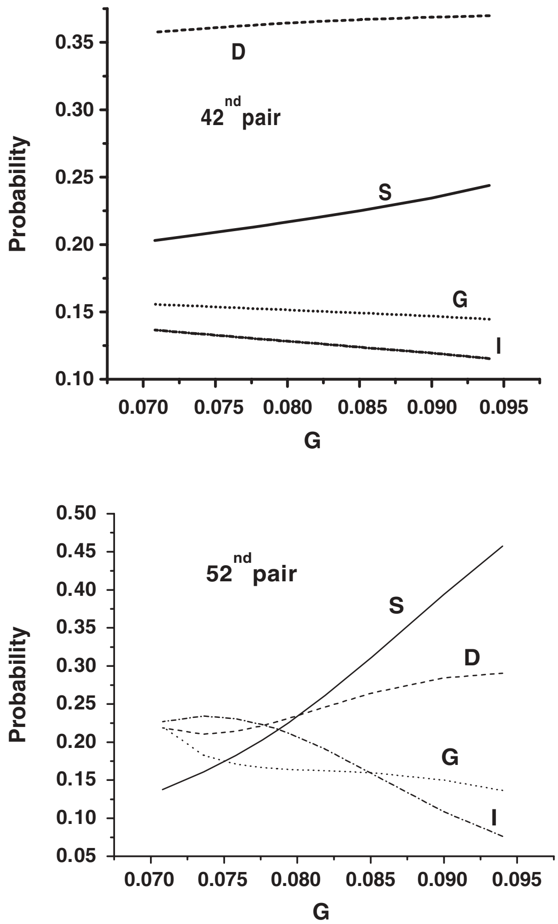

FIG. 2. Different angular-momenta probabilities for the Richardson neutron 42nd pair (upper figure)and for the Richardson neutron 52nd pair (lower figure) of the ^{174}Yb as a function of the strength of the pairing interaction.

IV. APPLICATIONS TO SOME REALISTIC CASES

To avoid confusions we summarize the calculation of the single-particle Nilsson basis that was used in the present calculation. We start considering a set of single particle levels calculated from a spherical harmonic oscillator with a strong spin orbit coupling where we added corrections for the centrifugal force and for proton-neutron asymmetry [2]. The wave functions are the ones of the harmonic oscillator and for each set of quantum numbers n, j, l, m, the energies (degenerated in the magnetic quantum number), are given by the following formula:

$$e_{njl} = \left\{(N+3/2) - \mu\left[l(l+1) - \frac{N(N+3)}{2}\right] - \kappa l\right\}\hbar\omega$$

for $j = l + 1/2$,

$$e_{njl} = \left\{(N+3/2) - \mu\left[l(l+1) - \frac{N(N+3)}{2}\right] - \kappa(l+1)\right\}\hbar\omega \quad \text{for} \quad j = l - 1/2, \tag{20}$$

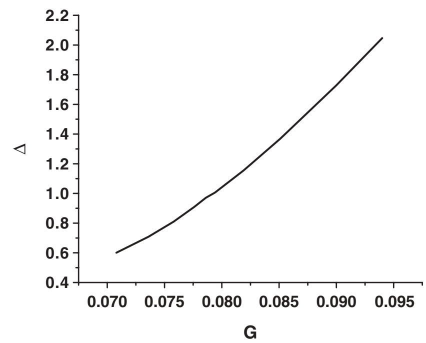

FIG. 3. Behavior of the gap Δ as a function of the pairing strength G calculated in the ^{174}Yb nucleus.

where $N = 2n + l$ is the principal quantum number and the parameters have been fixed for ^{174}Yb (in MeV):

$$\hbar\omega = 41A^{-1/3}\left(1 + \frac{A-2Z}{3A}\right),$$
$$\kappa = 0.06366 \; \mu = 0.02606, \tag{21}$$

for neutrons.

With this single-particle basis, including up to $N = 9$ we calculate the Nilsson single-particle basis diagonalizing a Hamiltonian with a quadrupole interaction of the form:

$$\langle j_1 m | H_{\text{Nilsson}} | j_2 m\rangle = e_{j_1,m}\delta_{j_1,j_2} - \beta\langle j_1 m | Q_{20} | j_2\rangle, \tag{22}$$

where m is the magnetic quantum number, conserved in the diagonalization, and j takes into account the rest of the quantum numbers of the level n, j, l. The quadrupole operator is the normal one:

$$Q_{20} = r^2 Y_{20}(\theta, \phi), \tag{23}$$

and the parameter β is related to the deformation parameter δ by the equation

$$\beta = \frac{1}{3}\sqrt{\frac{16\pi}{5}}\delta. \tag{24}$$

From the diagonalization of Eq. (22) we obtain the Nilsson eigenfunctions and the energy eigenvalues ϵ_{i,m_i} that will be our single particle Hamiltonian.

For each deformation of the Nilsson Hamiltonian, we add a pairing interaction and we proceed to solve the Richardson equations for 52 neutron pairs. The equations are solved

TABLE I. Probabilities of different angular momenta J of the BCS solutions obtained with the indicated value of the deformation parameter δ.

δ	$J=0$	$J=2$	$J=4$	$J=6$	$J=8$
0.000	1.000	0.000	0.000	0.000	0.000
0.100	0.973	0.026	0.001	0.000	0.000
0.125	0.961	0.037	0.002	0.000	0.000
0.150	0.948	0.048	0.003	0.001	0.000
0.200	0.924	0.068	0.006	0.002	0.000
0.250	0.902	0.086	0.008	0.003	0.001
0.300	0.879	0.103	0.012	0.004	0.001

TABLE II. Probabilities of different angular momenta J of the 42nd Richardson's pair for the indicated value of the deformation parameter δ.

δ	$J = 0$	$J = 2$	$J = 4$	$J = 6$	$J = 8$	$J = 10$	$J = 12$	$J = 14$
0.001	0.993	0.007	0.000	0.000	0.000	0.000	0.000	0.000
0.100	0.243	0.370	0.244	0.123	0.020	0.001	0.000	0.000
0.125	0.198	0.371	0.258	0.134	0.036	0.003	0.000	0.000
0.150	0.162	0.360	0.267	0.150	0.055	0.006	0.000	0.000
0.200	0.154	0.474	0.280	0.073	0.017	0.003	0.000	0.000
0.250	0.216	0.364	0.152	0.129	0.107	0.029	0.004	0.000
0.300	0.129	0.109	0.200	0.351	0.158	0.040	0.011	0.002

starting with a rather large value of G (of the order of 1 MeV) where the solution for the ground sate has a simple structure: all pairs have an energy with a real part smaller than the smaller single pair energy. Displaying the real and imaginary part of the energies, in the complex energy-plain E, we produce a simple pattern where all the energies have a nonzero imaginary part and form a quadratic curve. From this starting point, G is decreased by successive small amounts and the solution, corresponding to the ground sate, can be clearly followed.

It can be shown that if two of the energies (complex conjugates) have small imaginary parts and equal real parts close to twice one of the single particle energies, for a smaller value of G, they split into two solutions with real energies, one slightly smaller and the other slightly larger than twice the single particle energy. These energies remain real for smaller values of G and get closer to twice the single particle energy. We used this fact to check that, for G going to zero, the lowest energy state obtained corresponds to the filling of the 52 lowest levels given by the Nilsson Hamiltonian.

In Fig. 1 we display the energy of the neutron Richardson's pairs of ^{174}Yb for different deformations. The strength of the pairing interaction was chosen in such a way that the gap parameter, defined in terms of the occupation probabilities of the levels, was equal to 1 MeV [see Eq. (12)]. It is clear from the figure that the energies of the Richardson's pairs can be separated into two different groups: on one side there are strongly bound pairs with real energies or with very small imaginary parts and correspond basically to pairs of nucleons in particular Nilsson levels. These pairs usually are far away from the Fermi energy and are not affected much by the pairing interaction. They usually correspond to nonactive particles that can, in principle, be disregarded in studying the low energy spectra of the nuclei. On the other hand there are levels close to the Fermi energy that try to develop a pattern in the E-plane similar to the large G pattern. In Fig. 1 we show that the deformation has a very strong influence in the behavior of these pairs.

One of the purposes of the present study is to look at the angular momentum decomposition of these last pairs. In order to have a reference point, we calculate, using the BCS treatment, the angular momentum decomposition of the Cooper pair related to BCS ground state, using the procedure given in Ref. [13]. In Table I the probabilities corresponding to different deformations obtained with BCS are shown. It is noticeable that the amount of S pairs increases as the deformation decreases and that the S and D pairs can describe almost completely the structure of the BCS pair.

In Tables II and III we display the angular momentum decomposition for two of the Richardson's pairs for different deformations. Table II corresponds to the 42nd pair while Table III display the same results for the 52nd pair. For zero deformation the S pair dominates completely but as the deformation is increased, the higher angular momenta begin to become important. Even more, for deformations $\delta = 0.15$–0.3 the weight of angular momenta $J = 4$ to $J = 10$ are comparable with the lower ones S and D.

It is interesting to study the influence of the pairing strength on the probability of obtaining different angular momentum. In Fig. 2 we display these probabilities for the 52nd and the 42nd pairs as functions of the pairing strength, and in Fig. 3 we display the values obtained for Δ using these strengths. It is shown that even if the influence of the S boson increases by a small amount as G is increased the situation does not change too much.

TABLE III. Probabilities of different angular momenta J of the 52nd Richardson's pair for the indicated value of the deformation parameter *delta*.

δ	$J = 0$	$J = 2$	$J = 4$	$J = 6$	$J = 8$	$J = 10$	$J = 12$	$J = 14$
0.001	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.100	0.543	0.298	0.116	0.035	0.006	0.001	0.000	0.000
0.125	0.430	0.304	0.164	0.076	0.018	0.006	0.002	0.000
0.150	0.347	0.284	0.188	0.124	0.033	0.017	0.006	0.000
0.200	0.277	0.248	0.177	0.191	0.051	0.041	0.013	0.001
0.250	0.226	0.231	0.164	0.212	0.071	0.070	0.023	0.003
0.300	0.139	0.221	0.227	0.196	0.094	0.086	0.031	0.005

TABLE IV. Absolute values of the overlaps between the same component of angular momenta J, between some pairs, ordered for increasing energies, against the one near the Fermi energy (52) of the ^{174}Yb. The deformation parameter we have taken, as an example, is $\delta = 0.25$. The angular momenta are displayed in the columns while the pairs involved (M_i) are shown in the files.

$\langle M_1 \vert 52\rangle$	$J = 0$	$J = 2$	$J = 4$	$J = 6$	$J = 8$	$J = 10$	$J = 12$
42–52	0.423	0.336	0.231	0.049	0.215	0.102	0.156
43–52	0.311	0.414	0.277	0.048	0.385	0.300	0.366
44–52	0.663	0.583	0.355	0.163	0.277	0.280	0.415
45–52	0.469	0.317	0.125	0.301	0.347	0.556	0.549
46–52	0.165	0.687	0.241	0.293	0.396	0.331	0.652
47–52	0.415	0.156	0.275	0.414	0.302	0.203	0.741
48–52	0.737	0.342	0.322	0.722	0.400	0.171	0.731
49–52	0.476	0.324	0.392	0.174	0.395	0.736	0.885
50–52	0.642	0.723	0.736	0.718	0.609	0.924	0.963
51–52	0.226	0.335	0.686	0.202	0.106	0.888	0.935

It is worthwhile to note that even if it is possible to explain, in a phenomenological way, the behavior of deformed nuclei using only S and D bosons well [6,7], the exact calculation with realistic parameters used in the present paper suggests that the inclusion of pairs of fermions coupled to higher angular momenta will be mandatory in order to obtain a microscopic description of those nuclei. Additionally, we want to call to attention the fact that, even if the BCS ground state is a very good description of nuclei near sphericity, it is quite different from the exact solution, for deformed ones.

Additionally, it should be mentioned that the different pairs of the Richardson's exact solution do not have similar structures regarding the angular momenta decomposition. We have displayed in Table IV the overlaps between different pairs (from 42 to 51) against the one nearest the Fermi energy (52). As the overlaps are complex numbers, we show in the table only their absolute values. It is clear from the overlaps obtained that they are neither similar nor follow any special trend. Therefore, in this solution, it is not possible to speak about a single S, D, G boson, because their proportions are changing from one pair to the other. In consequence, even if we consider that higher angular momenta are necessary for a description of deformed nuclei using reasonable interactions, it should not be directly compared to the amount of J angular momentum of the Richardson's pairs with the J boson of any bosonic approximation that use only one type of bosons in their descriptions.

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