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Exact Diagonalisation of Pairing Interactions for Protons and Neutrons in j-j Coupling. I. Even Nuclei, $d_{3/2}$ — $f_{7/2}$ Shells

Dokładna diagonalizacja oddziaływania pairing dla protonów i neutronów w sprzężeniu j-j. I. Jądra parzyste, powłoki $d_{3/2}$ — $f_{7/2}$

Точная диагонализация парного взаимодействия для протонов и нейтронов в связи j—j. I. Нечетные ядра, уровни $d_{3/2}$—$f_{7/2}$

Pairing interaction as a model residual interaction in the frame of nuclear shell model has a rather long history. Racah [1] gave an exact formulae for pairing energy in a degenerated case in L-S coupling. So-called seniority scheme in L-S was generalised by Flowers [2], and Edmonds and Flowers [3] for j-j coupling where the same concept was introduced. Application of unitary, orthogonal (L-S) and symplectic (j-j) groups enlarged and made easier theoretical treatment. There were, however, some limitations imposed by the mathematical apparatus of group theory. Every shell has to be connected with a group of different dimension and this does not allow to consider more than one degenerated level. Since 1958 the situation has been improved as the well-working superconductivity approximation, introduced at first by Bardeen, Cooper and Schrieffer [4] in a solid state theory, has been applied to nuclear theory by Mottelson [5], Bielajev [6] and others. This approximation works, however, for one kind of nucleons only. A further progress was made when the so-called quasi-spin method was applied to the theory of pairing interactions. Wada, Takano and Fokuda [7] were the first to notice the simple commutation relations among the fermion creation and annihilation operators taken in second order combinations. This was a clue for development of the quasi-spin method.

Since then the quasi-spin formalism together with orthogonal groups connected with it has been widely exploited. Identification of groups generated by infinitesimal operators taken from the pairing Hamiltonian was done in the works of Ichimura [8—9], Lipkin [10] and of [11—12]. Calculation of matrix elements of generators in the constructed basis was done by Hecht [13]. The same but for special representations in which physical operators with good quantum numbers were used, was performed in the works [14—15]. Equivalent results but with the use of a different method were obtained by Richardson [16—17]. The great number of published papers devoted both to mathematical and physical applications of the quasi-spin method have not been mentioned here. From the point of view of the present work it has to be stressed that Kerman et al. [18] was the first to calculate the energy levels for several one-particle shells with one kind of nucleons correlated by the pairing forces. The similar problem but for two shells only was considered in the paper [19]. Quite recently Hecht and Pang [20] have overcome mathematical difficulties in the R_8 group connected with pairing interactions in *L-S* coupling and have been able to calculate the pairing energy for the system of protons and neutrons and for several shells in *L-S* coupling.

The present work deals with the pairing interactions for both protons and neutrons in some realistic case of two shells: $3/2^+$ and $7/2^-$. Pairing interactions in *j-j* coupling work only for two-particle state with $T=1$, excluding, by the symmetry principle, states with $T=0$. In that respect those interactions can be placed between two extremes: 1) interactions without correlations proton-neutron and 2) interactions with correlations and with $T=0;1$ so, as it is in *L-S* coupling. In this paper we have taken an even number of protons and neutrons with seniority zero. For such representations only three quantum numbers are needed for classifying the states under R_5 [15] symmetry specific for *j-j* coupling. The set of physical quantum numbers consists of the isospin T, its third component T_0 and the number of nucleons modified by a constant.

In the first part of the work we have briefly presented the obtained results and in the second part we have dealt with some details of the group-theoretical classification of representations considered in this paper.

I. DIAGONALISATION OF THE PAIRING HAMILTONIAN

We follow here the notation of the paper [11].

Let us consider n nucleons in a certain configuration with seniority zero on the $j_1={}^3/_2$ and $j_2={}^7/_2$ levels separated by the energy ε. If we take the energy of the system relatively to the lower one-particle level j_1, the pairing Hamiltonian for both, protons and neutrons, will have the form

$$H=\sum_{m_2}\varepsilon\, a^{+}_{j_2m_2}a_{j_2m_2}-G\sum_{jj'}\left\{\frac{1}{2}\left(S^{np}_{+}\right)_{j}\left(S^{np}_{-}\right)_{j'}+\left(S^{n}_{+}\right)_{j}\left(S^{n}_{-}\right)_{j'}+\left(S^{p}_{+}\right)_{j}\left(S^{p}_{-}\right)_{j'}\right\} \quad (1)$$

where $S\pm$ operators are suitable quasi-spin operators, and j, j' take on the values j_1, j_2. The first part of the Hamiltonian has zero-matrix elements between states of different configurations. Diagonal elements of this part are simply equal to $n_2\varepsilon$, where n_2 is the number of particles on the level j_2.

The matrix elements of the operators $S\pm$ have been calculated in the work [15] for a given j with the help of orthogonal group R_5 in the five-dimensional abstract space. In the case of two j's we face the problem of the Kronecker product of two irreducible representations of the R_5 group. Taking as a basis the simple products of states

$$|nTTo>_{j1}|nTTo>_{j2}\equiv|(nTTo)_{j1}(nTTo)_{j2}> \quad (2)$$

we can easily calculate matrix elements of all the products S_+S_-. The dimension of the matrix H depends on the total $n=n_1+n_2$. Table 1 gives these numbers for several discussed cases.

Table 1. Dimensions of the matrix H for given values of the number of particles

Total n	4	6	8	10	12
dim. H	7	11	21	24	30

It is, however, more convenient to change the basis, taking as good quantum numbers the total isospin T, its third component T_0, and isospins T_1, T_2 for j_1 and j_2, respectively. The transformation can be done with the help of Clebsch-Gordan coefficients:

$$|n_1n_2(j_1j_2);T_1T_2;TT_0>=\sum_{T_{01}\,T_{02}}(T_1T_{10};T_2T_{20}|TT_0)\times|(nTT_0)j_1(nTT_0)j_2> \quad (3)$$

The transformation (3) gives us two advantages. As the matrix elements of H are equal to zero between the states of different total T, the problem of a given number of particles is divided into several problems of fixed T. This allows to assign to each calculated energy the state of a given isospin.

The Hamiltonian H is invariant under the transformation of the orthogonal isospin group R_3. Consequently, the energies do not depend

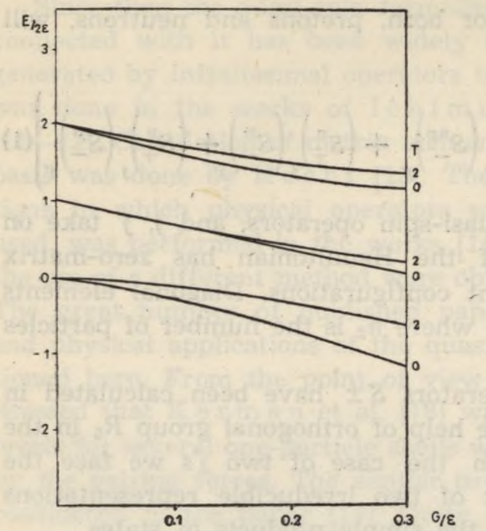


Fig. 1. Energies of the ground and excited states for four nucleons on $j_1=3/2$ and $j_2=7/2$ levels correlated by pairing forces, as functions of the strength parameter G. ε is one particle energy of the 7/2 level relatively to the 3/2 level

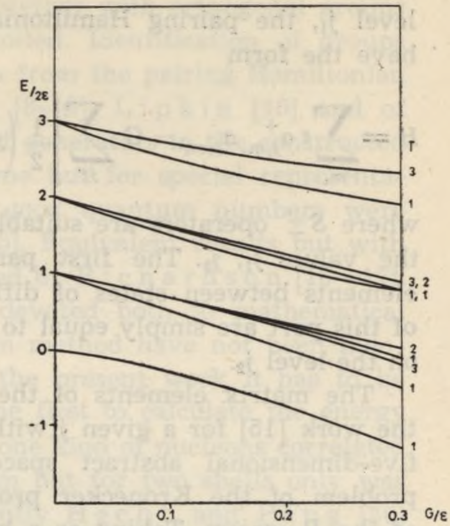


Fig. 2. Energies of the ground and excited states for six nucleons. For explanation see Fig. 1

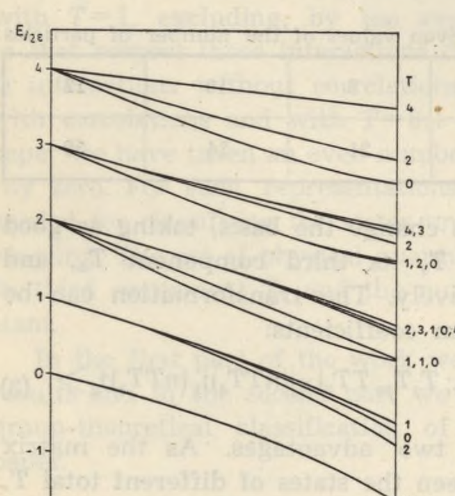


Fig. 3. Energies of the ground and excited states for eight nucleons. For explanation see Fig. 1

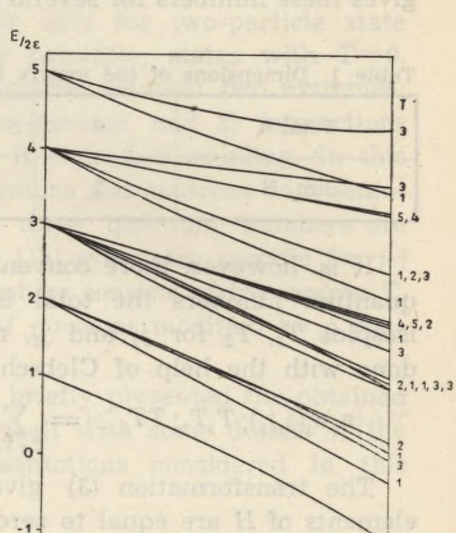


Fig. 4. Energies of the ground and excited state for ten nucleons. For explanation see Fig. 1

Table 2. Eigen-vectors of four nucleons with $T = 0$. The last three columns give the expansion coefficients in the base $| n_1T_1;\ n_2T_2;\ T>$ as functions of the strength parameter G and the eigen-values E

G/ε	$E/2\varepsilon$	$\|40;\ 00;\ 0>$	$\|21;\ 21;\ 0>$	$\|00;\ 40;\ 0>$
	−0.138	0.993	−0.113	0.020
0.05	0.850	0.113	0.987	−0.113
	1.787	0.007	0.113	0.994
	−0.301	0.975	−0.223	0.026
0.1	0.700	0.223	0.946	−0.236
	1.602	0.027	0.236	0.971
	−0.700	0.909	−0.406	0.096
0.2	0.378	0.402	0.789	−0.464
	1.322	0.113	0.460	0.881
	−1.177	0.829	−0.528	0.184
0.3	0.028	0.516	0.599	−0.612
	1.149	0.213	0.603	0.769

Table 3. Eigen-vectors of four nucleons with $T = 2$ (see Table 2)

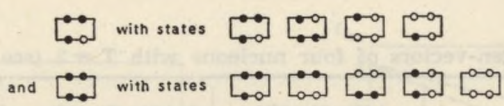
G/ε	$E/2\varepsilon$	$\|42;\ 00;\ 0>$	$\|21;\ 21;\ 0>$	$\|00;\ 42;\ 0>$
	−0.056	0.997	0.078	0.0035
0.05	0.848	−0.078	0.993	0.086
	1.858	−0.0032	0.086	−0.996
	−0.125	0.985	0.165	0.016
0.1	0.695	0.173	−0.971	−0.167
	1.729	0.013	−0.167	0.986
	−0.323	0.915	0.397	0.080
0.2	0.410	0.401	−0.865	−0.303
	1.513	0.051	−0.309	0.950
	−0.620	0.786	0.592	0.179
0.3	0.181	0.609	−0.690	−0.391
	1.339	0.107	−0.415	0.903

on the total T_0 of the system with protons and neutrons with fixed T, within a given irreducible representation of the R_5 group. This means that for a given T there are $2T+1$ degenerated in energy states of different T_0.

In Fig. 1—4 there are given the calculated energies for the strength parameter G (in unit ε) equal to 0.05; 0.1; 0.2 and 0.3, and for the total number of particles n=4, 6, 8, 10. The calculations have been done on the computer Odra 1013 in the Computer Center at M. Curie-Skłodowska University in Lublin. There have been also calculated the state vectors belonging to energy levels. They are the linear combinations of the vectors given by (3) with the same total T but with different n_1T_1; n_2T_2. Using the shortened notation, namely $|n_1T_1, n_2T_2, T>$, we have presented in Table 2 and 3 the examples of state vectors for a fixed value of n and for several values of the G.

II. GROUP-THEORETICAL DISCUSSION

Irreducible representations of the R_5 group are denoted by $D(\lambda_1\lambda_2)$ where λ_1 and λ_2 stand for the numbers of two fundamental representations of the group (see for example [21]). According to the results of [15], these fundamental representations can be drawn, in quasi-spin picture, as



where each block consists of four one-particle states with the same $|m|$.

Sets of states on the 3/2 and 7/2 levels form bases for irreducible representations $D(0.2)$ and $D(0.4)$ in the case of seniority zero. Mixed states of both 3/2 and 7/2 form the basis for the direct product $D(0.2) \oplus D(0.4)$ which is presented in [15]:

$$D(0.2) \oplus D(0.4) = D(0.2) \oplus D(0.4) \oplus D(0.6) \oplus D(2.2) \oplus D(2.4) \oplus D(4.2) \quad (4)$$

The dimension of every irreducible representation is given by

$$N = \frac{1}{6}\left(\lambda_1 + 1\right)\left(\lambda_2 + 1\right)\left(\lambda_1 + \lambda_2 + 2\right)\left(\lambda_1 + 2\lambda_2 + 3\right) \quad (5)$$

Equalizing the dimensions according to (4) and (5) one gets
$14 \times 55 = 14 + 55 + 140 + 81 + 260 + 220 = 770.$

With the help of the rule of adding two isospins we have found the values of the total T for each irreducible representation under consideration (Table 4).

Table 4. Allowed values of T for particular representations $D\ (\lambda_1, \lambda_2)$ of the R_5 group

$D\ (\lambda_1, \lambda_2)$	Number of particles	$\pm$ So	T
(0,2)	0; 8	2	0
	2; 6	1	1
	4;	0	0, 2
(0,4)	0; 16	4	0
	2; 14	3	1
	4; 12	2	0, 2
	6; 10	1	1, 3
	8;	0	0, 2, 4
(0,6)	0; 24	6	0
	2; 22	5	1
	4; 20	4	0, 2
	6; 18	3	1, 3
	8; 16	2	0, 2, 4
	10; 14	1	1, 3, 5
	12;	0	0, 2, 4, 6
(2,2)	2; 14	3	1
	4; 12	2	0, 1, 2
	6; 10	1	1 (2x), 2, 3
	8;	0	0, 1, 2 (2x), 3
(2,4)	2; 22	5	1
	4; 20	4	0, 1, 2
	6; 18	3	1 (2x), 2, 3
	8; 16	2	0, 1, 2 (2x), 3, 4
	10; 14	1	1 (2x), 2, 3 (2x), 4, 5
	12;	0	0, 1, 2 (2x), 3, 4 (2x), 5
(4,2)	4; 20	4	2
	6; 18	3	1, 2, 3
	8; 16	2	0, 1, 2 (2x), 3, 4
	10; 14	1	1 (2x), 2 (2x), 3 (2x), 4
	12;	0	0, 1, 2 (3x), 3 (2x), 4

The number S_0 is equal, following [11], to $1/2\,(n\text{-}\Omega)$.

As an example for further discussion, let us consider a case with $n=6$ particles. States with six particles can be composed of the states of both $D(0.2)$ and $D(0.4)$ representations given in Table 5.

Table 5. Mixed states with six particles on the 3/2 and 7/2 levels

D (0.2)		D (0.4)		Total T
n_1	T_1	n_2	T_2	
6	1	0	0	1
4	0; 2	2	1	1, 1, 2, 3
2	1	4	0; 2	1, 1, 2, 3
0	0	6	1; 3	1, 3

Every state has the total S_0 equal to minus three. The problem is an eleven-dimensional one. If we, however, couple the states to the total T, the matrix elements between the states of different T will vanish, and the whole problem will consist of three problems with $T=1$ (6-dimensional), $T=2$ (2-dimensional), and $T=3$ (3-dimensional). We want to assign to each state its group-theory classification numbers. This means that we have to divide the eleven states into states belonging to a given irreducible representation of the Clebsch-Gordan series (4). Taking the states of Table 4 with six particles we get, however, the set of states with different T, as compared to the states given in Table 5. This interesting disagreement is caused by the fact that the pairs of particles with seniority equal two, and with reduced isotopic spin equal to zero are like scalars under transformations of the orthogonal group R_5 [15], and may be added to the states of a given irreducible representation without any change in transformational properties. This means that the number of particles is not a good criterion of choosing the proper states from Table 4. On the other hand the good and additive quantum number is given by S_0. Taking the states from Table 4 with $S_0=-3$ we get the right set of the total T. In order to retain the total number of particles we have to add to the representations, the pairs of particles with $s=2$; $t=0$, in such a way as to obtain a number of particles equal to six. Following the above considerations we divide the set af the total T among the irreducible representations of (4) (Tables 6). Calculated energies of all the eleven states have to be divided into states belonging to the given irreducible representations according to Table 6.

Table 6. Classification of states of six nucleons according to (4)

(λ_1, λ_2)	s	t	T
(0, 4)	4	0	1
(0, 6)	0	0	1, 3
(2, 2)	6	1	1
(2, 4)	2	1	1, 1, 2, 3
(4, 2)	4	2	1, 2, 3

Let us begin with the degenerated case when G is so great that we can abandon the value of ε as compared with G. In such a case the energy is given by the exact formulae [11]:

$$E = -\frac{G}{4}\left\{\left(n-s\right)\left(2\Omega + 2 - \frac{n}{2} - \frac{s}{2}\right) - 2T(T+1) + 2t(t+1)\right.$$

where $\Omega = \Omega_1 + \Omega_2$

and $\Omega_1 = j_1 + \frac{1}{2}$ $\Omega_2 = j_2 + \frac{1}{2}$

Taking the quantum numbers from Table 6 we obtain the levels of all the states (Fig. 5).

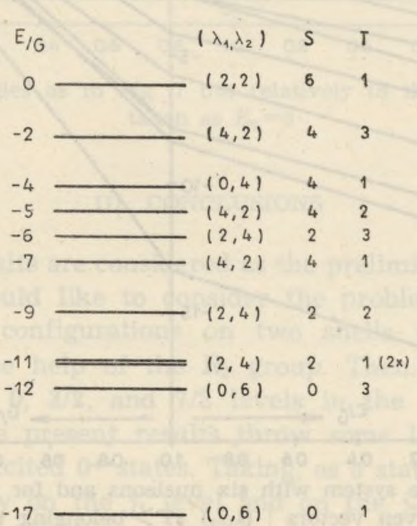


Fig. 5. Ground and excited states with six particles on 3/2 and 7/2 levels in the degenerated case of $\varepsilon/G \to 0$

Taking as a parameter the $\frac{E}{G}$ (or $\frac{G}{E}$) in a range (o, ∞), we obtain the energies of excited levels as functions of the parameter. The starting points of curves are taken from Fig. 5. On the other ends of curves $\frac{E}{G} \to \infty$) we have also well known points, because for the case of $G=0$ we have only the single-particles excitation energies (Fig. 6).

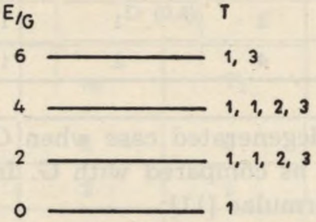


Fig. 6. Energies and isotopic spins for $G=0$ in the case of six particles on the levels 3/2 and 7/2

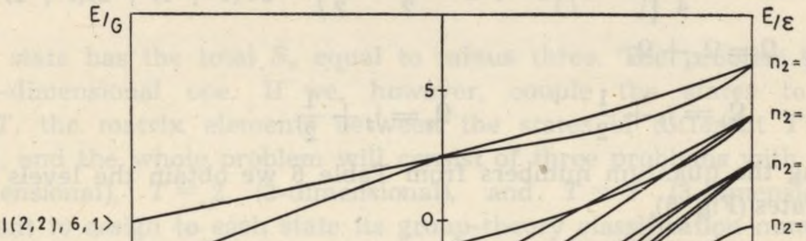


Fig. 7. Energies for the system with six nucleons and for $0 \leqslant G < \infty$. On the left hand side there are given vectors $|\ (\lambda_1\lambda_2)\ sT >$ belonging to particular states, and on the right hand side, for $G=0$ there are given pure states with $n_2=0$, 2, 4, and 6 nucleons on the higher 7/2 level

Between these two extremes we have calculated the energies for several points which are given in Fig. 7—8.

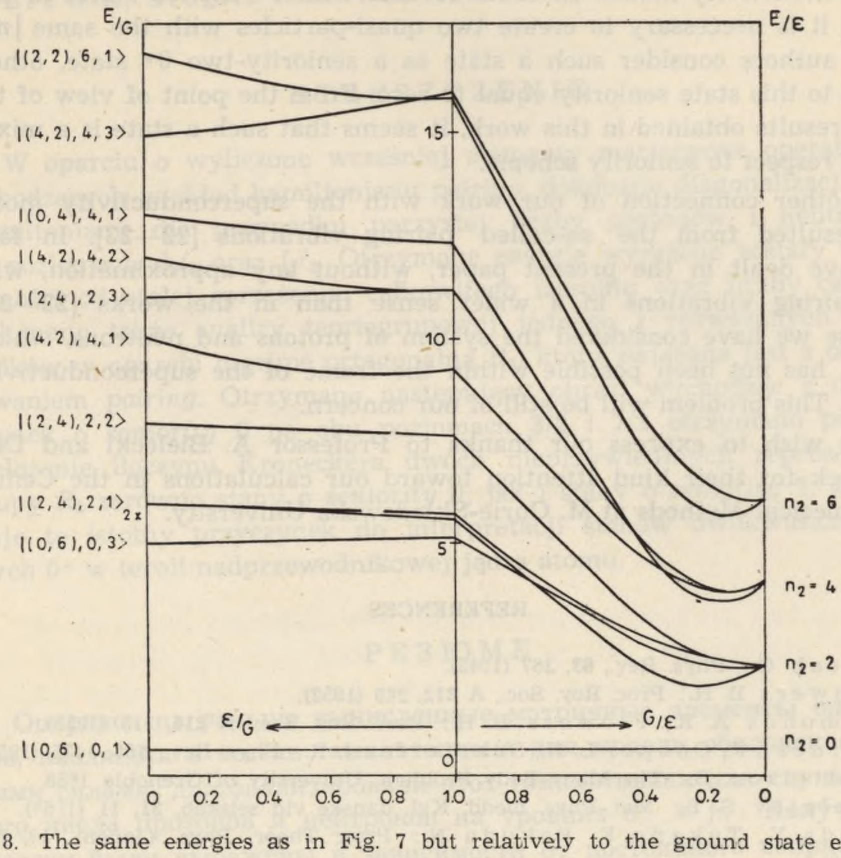


Fig. 8. The same energies as in Fig. 7 but relatively to the ground state energy taken as $E_0 = 0$

III. CONCLUSIONS

The obtained results are considered as the preliminary ones to a large--scale work. We would like to consider the problem more thoroughly taking all possible configurations on two shells under the seniority scheme and with the help of the R_5 group. Then, it will be possible to interpret certain 0, 3/2, and 7/2 levels in the discussed region of nuclei. However, the present results throw some light on the controversial problem of excited 0^+ states. Taking, as a starting point, seniority zero states separately on the j_1 level and on the j_2 level, and forming linear combinations of such seniority-zero states, we have obtained not only seniority-zero product, but also the states with seniority 2, 4, 6, ...

This result obtained without any approximation may explain contradictory remarks concerning two quasi-particle excited states within the superconductivity model. In order to deal with 0^+ excited states in this model it is neccessary to create two quasi-particles with the same $|m|$. Some authors consider such a state as a seniority-two 0^+ state, others assign to this state seniority equal to zero. From the point of view of the exact results obtained in this work, it seems that such a state is a mixed one in respect to seniority scheme.

Another connection of our work with the superconductivity model has resulted from the so-called pairing vibrations [22—23]. In fact, we have dealt in the present paper, without any approximation, with the pairing vibrations in a wider sense than in the works [22—23], because we have considered the system of protons and neutrons, which, so far, has not been possible within the frame of the superconductivity model. This problem will be still of our concern.

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STRESZCZENIE

W oparciu o wyliczone wcześniej elementy macierzowe operatorów, wchodzących w skład hamiltonianu *pairing*, dokonano diagonalizacji tego hamiltonianu dla przypadku parzystej liczby protonów i neutronów na poziomach $d_2/_3$ oraz $f_7/_2$. Otrzymane energie wyrażone zostały w zależności od stałej sprzężenia, całkowitego izospinu oraz liczby cząstek. Dokonano także analizy teoriogrupowej jednego z rozważanych przypadków w oparciu o grupę ortogonalną R_5, która związana jest z oddziaływaniem *pairing*. Otrzymano następujący obraz: wychodząc z układu cząstek o *seniority* 0 na obu poziomach 3/2 i 7/2 otrzymano poprzez rozłożenie iloczynu Kroneckera dwóch nieprzywiedlnych reprezentacji grupy R_5 zarówno stany o *seniority* 0, jak i stany o *seniority* 2, 4, 6, ... Daje to istotny przyczynek do interpretacji stanów dwukwasicząstkowych 0^+ w teroii nadprzewodnikowej jądra atomu.

РЕЗЮМЕ

Опираясь на раньше вычисленные матричные элементы операторов, входящих в состав гамильтониана для модели оболочек с парными силами, диагонализировали этот гамильтониан для случая четного числа протонов и нейтронов на уровнях $d_{3/2}$ и $f_{7/2}$. Полученные энергии были выражены в зависимости от постоянного сопряжения, полного изоспина и числа частиц. Провели также теоретически групповой анализ одного из исследованных случаев, используя ортогональную группу R_5. Получили следующее: исходя из системы частиц с сеньоритом 0 на уровнях 3/2 и 7/2, получили через разложение произведения Кронекера двух неприводимых представлений группы R_5, как состояния с сеньоритами 0, так и с сеньоритами 2, 4, 6 ... Это дает существенный дополнительный материал к вопросу интерпретации двуквазиочастичных состояний 0^+ в сверхпроводниковой теориядра.

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STRESZCZENIE

W oparciu o wyliczone wcześniej elementy macierzowe operatorów wchodzących w skład hamiltonianu pairing, dokonano diagonalizacji tego hamiltonianu dla przypadku parzystej liczby protonów i neutronów na poziomach $d_{3/2}$ oraz $f_{7/2}$. Otrzymane energie zostały w jawnej postaci wyrażone przez wartości całkowitego izospinu oraz liczby cząstek. Dołączono także analizę teoriogrupową jednego z rozwiązań przybliżonych w oparciu o grupę ortogonalną R_5, która związana jest z oddziaływaniem pairing. Otrzymano następujący obraz: wychodząc z układu cząstek o seniority 0 na obu poziomach 3/2 i 7/2 otrzymano poprzez rozłożenie iloczynu Kroneckera dwóch nieprzywiedlnych reprezentacji grupy R_5 zarówno stany o seniority 0, jak i stany o seniority 2, 4, 6. Daje to istotny przyczynek do interpretacji stanów dwuciałowo-cząstkowych 0^+ w teorii nadprzewodnikowej jądra atomu.

РЕЗЮМЕ

Опираясь на ранее вычисленные матричные элементы операторов, входящих в состав гамильтониана взаимодействия с парными силами, диагонализирован этот гамильтониан для случая четного числа протонов и нейтронов на уровнях $d_{3/2}$ и $f_{7/2}$. Полученные энергии были выражены в зависимости от полного изоспина и числа частиц. Проведен также теоретико-групповой анализ одного из приближенных решений с помощью ортогональной группы R_5. Получили следующую картину: исходя из системы частиц с сеньорити 0 на уровнях 3/2 и 7/2, получили через разложение произведения Кронекера двух неприводимых представлений группы R_5, как состояния с сеньорити 0, так и с сеньорити 2, 4, 6. Это дает существенный вклад в интерпретацию двухквазичастичных состояний 0^+ в сверхпроводниковой теории ядра.

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