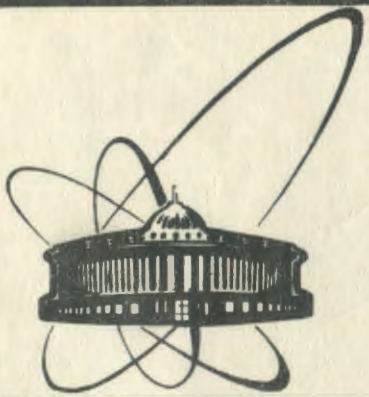

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NUMERICAL CALCULATIONS OF TRANSITIONAL NUCLEI.

1. NUCLODD - a Computer Program for Calculation of the Energies and Wave Functions of Odd Nuclei

1990

1. INTRODUCTION

The adequate description of transitional nuclei is a long standing problem in nuclear structure theory. One usefull approach for interpretation of odd-A nuclear system is proposed in the original work of Jolos /1/ in which the basis vectors for construction of the ground and excited state wave functions of odd (Z, N+1 or Z+1, N) nucleus are obtained by coupling of odd nucleon (in appropriate single-particle states) to some chosen even-even core states. This semi-microscopic version of Particle-Vibration Coupling (PVC) model, which incorporates both anharmonicities of the core vibrations and pairing effects in odd-nucleon motion, is used in the present computer program. It yields complete information about the particle-hole srtucture of the calculated states which one uses for further analysis of transition probabilities and static moments of the states. Several versions of the model are possible depending on which kind of core description is appropriate for calculated odd-system. In case, where the neighbouring even-even nuclei display features similar to those obtained by describing them in the frame of a particular limit of Intracting Boson Approach (IBA), the corresponding IBM-matrix elements are inserted as input parameters in the calculations of odd-nucleus. When the available experimental information about the collective features of the neighbouring even-even nuclei is inserted directly into calculations additionally to nuclear structure information, one can obtain information about the form parameters (or evolution of particular state structure changing Z or N) on the ground of subsequal model independent analysis (see Refs./2, 3/ and quotation therein).

2. BRIEF DESCRIPTION OF THE MODEL

The model has been described elswhere (see, for instence, Refs./1-3/) therefore we give here only a brief exposition.

The total Hamiltonian of the coupled system is

$$H = \sum_{jm} E_j a^+_{jm} a_{jm} - \frac{1}{4} QP \; P - \kappa \sum_{\mu} Q^+_{2\mu} Q_{2\mu} . \qquad (1)$$

The odd-nucleus states are chosen /1/ to be a superposition of the states $|InM, A \pm 2>$ of the adjacent even-even nuclei with $(A \pm 2)$ particles in the following way

$$|J_0 M_0, A+1> = \sum_{InMjm} \left(C^{J_0 M_0}_{Imjm} P^{J_0}_{Inj} a^{+}_{jm} |InM, A> - \right.$$

$$\left. - C^{J_0 M_0}_{Imjm} h^{J_0}_{Inj} \bar{a}_{jm} |InM, A+2> \right). \qquad (2)$$

Here $a^{+}_{jm}(a_{jm})$ are the creation (annihilation) operators of the nucleons in states with quantum number jm; InM label the core states and JM are the total angular momentum of odd-system and its z-component. The energies ϵ^{J}_{A+1} of the odd nucleus and the amplitudes p^{J}_{Inj} and h^{J}_{Inj} in eq.(2) can be obtained as a solution of closed set of equations, derived in Ref./1/

$$(\tilde{E}_j + E^{A}_{In}) p^{J_0}_{Inj} + \Delta^{A}_{In} h^{J_0}_{Inj} + \sum_{I'n'j'} \Gamma^{A}_{Inj, I'n'j'} p^{J_0}_{I'n'j'} = (\epsilon^{A+1}_{J} - \tilde{E}_0) p^{J_0}_{Inj},$$

$$(-\tilde{E}_j + E^{A+2}_{In}) h^{J_0}_{Inj} + \Delta^{A+2}_{In} p^{J_0}_{Inj} + \sum_{I'n'j'} \Gamma^{A+2}_{Inj, I'n'j'} h^{J_0}_{I'n'j'} = (\epsilon^{A+1}_{J} - \tilde{E}_0) h^{J_0}_{Inj}. \qquad (3)$$

Here Δ is the pairing gap; κ is the quadrupole copling constant, $\tilde{E}_j = E^{sp}_j - \lambda$.

The well-known problem of simultaneous calculation of both sets of states, with positive and negative parity, when states with J and J-1 follow the correct order, is solved in this version of the model by introducing additional term D

$$D = \kappa_D \sum_{\substack{I'n'j' \\ I''n''j''}} (-1)^{I'-I''} f(\epsilon_{j'}, \epsilon_{j''}) \begin{Bmatrix} j' & J & I' \\ \lambda & I & I'' \\ j' & j & \lambda \end{Bmatrix} q_{j'j''} q_{j''j} (Q^{coll}_2)_{II''} (Q^{coll}_2)_{I''I'} \qquad (4)$$

which corresponds to the exchange between the odd quasiparticle and quasiparticle which builds the quadrupole phonon.

3. STATIC MOMENTS AND TRANSITION RATES

The expressions used in obtaining the magnetic dipole moments μ^{J_k}, the electric quadrupole moment Q^{J_k} and the

M- and E-transition rates are as follows:

$$\mu^{J_k} \frac{eh}{2Mc} = -\sqrt{\frac{4\pi}{3}} C^{JJ}_{JJ10} \Big[\sum_{Injj'} \alpha_1(Injj') \chi_1(p^{J_k}, h^{J_k}) \langle j' || \mathfrak{M}(M1) || j \rangle + \tag{5}$$

$$+ \sum \alpha_2(Injj') \chi_2(p^{J_k}, h^{J_k}) \langle I'n' || \mathfrak{M}(M1) || In \rangle ,$$

$$Q_2^{J_k} = \sqrt{\frac{16\pi}{5}} C^{JJ}_{JJ20} \Big[\sum_{Injj'} \beta_1(Injj') \chi_3(p^J, h^J) \langle j' || \mathfrak{M}(E2) || j \rangle + \tag{6}$$

$$+ \sum_{In I'j'} \beta_2(Injj') \chi_4(p^J, h^J) \langle I'n' || \mathfrak{M}(E2) || In \rangle \Big] ,$$

$$B(\sigma L; J_1 \to J_2) = \Big[\sum_{Injj'} \gamma(Injj') \langle j' || \mathfrak{M}(\sigma L) || j \rangle \chi_5(p^J, h^J) + \tag{7}$$

$$+ \sum_{I'n'j} \gamma_2(I'n'j) * \chi_6(p^J, h^J) \langle I || \mathfrak{M}(\sigma L) || I \rangle .$$

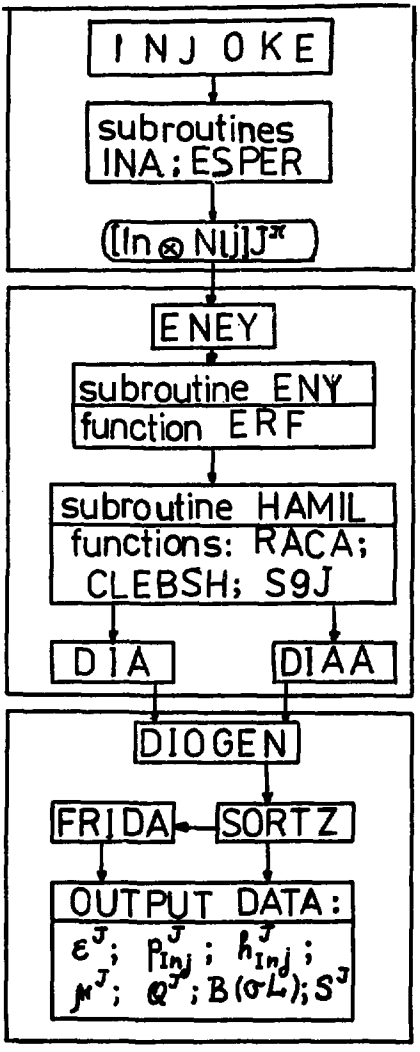
In Eqs.(5)-(7) there appear orbital and spin angular momentum g-factors for which quenching factors are easily inserted if necessary and the g-factor of the core is $g_p = Z/A$. The explicit form of the coefficients α, β, γ, χ see in the original publications /1,2/.

4. METHOD OF SOLUTION AND STRUCTURE OF THE PROGRAM

At the flow diagram (Figure), the particle core coupling program is presented.

The package INJOKE reads all input data (described below) and determins matrices dimensions for all calculated spins. It creates files in which for a treated nucleus this information can be saved.

The quadrupole field acting on the particle includes single-particle $q_{jj'} = \langle j || r^\lambda Y_\lambda || j' \rangle$ and collective $(Q_\pi^{coll})_{II'} \equiv \equiv \langle In || Q_\lambda || I'n' \rangle$ matrix elements which are calculated in package ENEY. It consists of subroutines ENY (reading the input data), ESPER, which calculates the quasiparticle energies and HAMIL, organizing the energy matrix H for further diagonalization. The vector-coupling coefficients, as well as single-particle matrix elements are obtained using additionally functions ERF, S9J, RACA, C1EBSH. Two different options are possible which correspond to two different kinds of H, created in this packge: one for rigorous diagonalization of matrix H and another, for matrix HH, in which the exchange effect (Eq.4)


INJOKE
subroutines
INA; ESPER
$([In \otimes N(j)]J^{\pi})$
ENEY
subroutine ENY
function ERF
subroutine HAMIL
functions: RACA;
CLEBSH; S9J
DIA
DIAA
DIOGEN
FRIDA
SORTZ
OUTPUT DATA:
ε^J; $P^J_{In_j}$; $h^J_{In_j}$;
μ^J; Q^J; $B(\sigma L)$; S^J

Figure

4

is taken into account. For all calculated spins J^{A+1} matrices H and HH are saved in a new created files DIA and DIAA, respectively, being as well input data for the next package DIOGEN. The two proposed options allow one to observe the influence of the exchange effect on the final results.

The calculation of the static moments and transition probabilities is carried out in the program FRIDA.

After diagonalisation of matrix H in subroutine DIO (based on Jackobi-method discussed elsewhere), the obtained eigenvalues and eigenvectors are ordered by subroutine SORTZ and printed as it is shown in tables 2,3.

5. THE INPUT DATA

All necessary initial information about the nucleus under consideration is presented in Table 1.

In section A are listed the parameters of the program:

- number of states to be calculated and of the ground state;
- codes for the options which calculates the energies and wave functions and transition probabilities and static moments;
- number of the single-particle (nb) and collective (na) states to be taken into account.

The description of the single-particle basis is included in section B. Here one inputs nb-times:

- Spin (j) - Energy (E_j) - Principale quantum number (N) - Parity (π) of the single particle state.

The description of the core is made in section C which reads:

- Spin (I) - Energy (E_{In} for A core) - Energy (E_{In} for A+2 core) - Parity (π) for na-collective states;
- the constants of the quadrupole and pairing interactions, the steps for their variation, chemical potential λ and the steps for its variation;
- Q_2-matrix elements between the states In and I'n' of the core, calculated before in an appropriate nuclear model.

The parameters for subroutine FRIDA are introduced in section F (not included in table 1).

6. DESCRIPTION OF THE OUTPUT

An example of an output set is given in Tables 2,3. The components of the wave functions normalized by the condition

Table 1. Input data for the program NUCLODD

section A				
6	2			
0.5	5.5			
1	1			
4	5			
section B				
0.1	0.1			
804.	818.			
0.5	-7200.	4	+1	
1.5	-6600.	4	+1	
2.5	-8800.	4	+1	
3.5	-9800.	4	+1	
5.5	-7000.	5	-1	
section C				
0	0.	0.		
2	604.	818.		
2	1167.	1551.		
4	1400.	1866.		
8086.	8049.	1000.	0.01	0.01 1
-6000.	-200.	1.0		
0.0	1.0	0.01	0.0	
1.0	-0.3	0.9	1.6	
0.01	0.9	0.3	0.0	
0.0	1.6	0.0	-0.3	
0.0	1.0	0.01	0.0	
1.0	-0.3	0.9	1.6	
0.01	0.9	0.3	0.0	
0.0	1.6	0.01	0.0	

Table 2. Part of the output data from the program NUCLODD. Wave function components for the states J=0.5

In x j	J= 5.000000E-01 eigenvectors for J = 0.5					
	particle- components					
0_1^+,0.5	.410	.063	-.014	.024	-.007	.002
2_1^+,1.5	-.384	.377	-.027	.009	-.004	.009
2_1^+,2.5	-.131	-.040	.029	.142	-.050	.003
2_1^+,1.5	-.162	.186	.431	-.013	.004	-.001
2_2^+,2.5	-.054	.008	.008	.086	.143	-.002
4_1^+,3.5	.067	-.071	.010	-.007	.006	.116
	hole- componente					
0_1^+,0.5	.737	.420	-.023	.239	-.068	.019
2_1^+,1.5	-.248	.764	-.224	.044	-.039	.126
2_2^+,2.5	-.158	-.145	.082	.860	-.408	.032
2_1^+,1.5	.049	.148	.868	-.063	.017	-.011
2_2^+,2.5	-.026	-.002	.006	.409	.896	-.015
4_1^+,3.5	.018	-.094	.036	-.032	.033	.984

Table 3. Output data from the program NUCLODD. Energies calculated for the states J=0.5; 1.5; 2.5; 3.5; 4.5; 5.5 (positive parity)

J= .5	208.014	878.579	1448.927	2614.483	3393.755	4669.562
J=1.5	.000	736.771	1051.469	1485.614	1846.898	2605.575
	3280.971	3505.113	3779.052	4325.346	4651.210	
J=2.5	687.566	904.263	1440.039	1600.143	1826.340	1982.312
	2718.302	3330.395	3527.918	3723.285	4252.382	4638.922
J=3.5	701.269	1382.770	1723.781	2203.364	2411.149	2618.693
	3338.345	3557.410	3739.671	4302.453	4656.490	
J=4.5	1640.794	1928.640	2716.945	3243.382	3391.821	3708.351
	4292.390	4663.731				
J=5.5	1655.781	3411.428	3643.319	4245.895	4639.551	

$(p^J_{Inj})^2 + (h^J_{Inj})^2 = 1$ are printed for every state J^{A+1} in column, following the coupling rule $[\,In \otimes nlj\,]\,J^{A+1}$. For brevity in table 2 only eigenvectors for J = 0.5 are shown. All eigenstates in order of growing energies are given in table 3.

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REFERENCES

1. Jolos R.V. - JINR Preprint P4-7967, Dubna, 1974.
2. Michailova M.M. et al. - J-Phys.G:Nucl.Phys., 1985, 12, p.L191.
3. Karloukovski V.I. et al. - Ann.Rep. de l'Universite Sofia 1987, v.78.

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